

## Supporting Information

# Robust Ru(II)–Bisbenzimidazole Catalyst Enables Sustainable and Scalable Valorization of Glycerol to Lactic Acid

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# 1. Determination of green metrics parameters

## 1.1 The CHEM21 green metrics toolkit

Supplementary information: Appendix 2		Summary of Zero Pass Metrics Toolkit																																		
Yield, conversion, selectivity, AE, RME																																				
Reactant (Limiting Reactant First)	Mass (g)	MW	Mol (M)	Catalyst	Mass (μmol)	Reagent	Mass (mg)	Reaction solvent	Volume (cm <sup>3</sup> )	Density (g ml <sup>-1</sup> )	Mass (g)	Work up chemical	Mass (g)	Workup solvent	Volume (cm <sup>3</sup> )	Density (g ml <sup>-1</sup> )	Mass (g)																			
Glycerol	12.60	92.09	0.14	Ru (PNP)	0.35	NaOH	560.00	NMP	8.00	1.03	8.24						0.00																			
											0.00						0.00																			
											0.00						0.00																			
											0.00						0.00																			
											0.00						0.00																			
											0.00						0.00																			
											0.00						0.00																			
<b>Total</b>	<b>12.60</b>	<b>92.09</b>			<b>0.35</b>		<b>560.00</b>				<b>8.24</b>		<b>0.00</b>				<b>0.00</b>																			
$AE = \frac{\text{molecular weight of product}}{\text{total molecular weight of reactants}} \times 100$ $RME = \frac{\text{mass of isolated product}}{\text{total mass of reactants}} \times 100$																																				
<table border="0"> <tr> <td>Yield</td> <td>68.6</td> <td>Flag</td> <td>68.6</td> </tr> <tr> <td>Conversion</td> <td>100.0</td> <td></td> <td>100.0</td> </tr> <tr> <td>Selectivity</td> <td>68.6</td> <td></td> <td>68.6</td> </tr> <tr> <td>AE</td> <td>97.8</td> <td></td> <td></td> </tr> <tr> <td>RME</td> <td>67.1</td> <td></td> <td></td> </tr> </table>																	Yield	68.6	Flag	68.6	Conversion	100.0		100.0	Selectivity	68.6		68.6	AE	97.8			RME	67.1		
Yield	68.6	Flag	68.6																																	
Conversion	100.0		100.0																																	
Selectivity	68.6		68.6																																	
AE	97.8																																			
RME	67.1																																			
<table border="0"> <tr> <td>Product</td> <td>mass (g)</td> <td>mw</td> <td>mol (M)</td> </tr> <tr> <td></td> <td>8.450</td> <td>90.080</td> <td>0.0938055</td> </tr> <tr> <td>Unreacted limiting reactant</td> <td>mass</td> <td></td> <td></td> </tr> </table>																	Product	mass (g)	mw	mol (M)		8.450	90.080	0.0938055	Unreacted limiting reactant	mass										
Product	mass (g)	mw	mol (M)																																	
	8.450	90.080	0.0938055																																	
Unreacted limiting reactant	mass																																			
<b>Solvents (Zero Pass)</b>																																				
<b>Highly hazardous solvents (Red flag for any of the following)</b>																																				
Et <sub>2</sub> O, Benzene, CCl <sub>4</sub> , chloroform, DCE, nitromethane, CS <sub>2</sub> , HMPA																																				
<b>List Highly Hazardous Solvents Below</b>																																				
None																																				
<b>Health and Safety (Zero Pass)</b>																																				
<b>Health &amp; safety (Red flag for any of the following)</b>																																				
<b>List substances plus the red flagged H-codes below</b>																																				
Highly explosive	H200, H201, H202, H203		None																																	
Explosive thermal runaway	H240		None																																	
Fatally toxic	H300, H310, H330		None																																	
Mutagenic	H350		None																																	
Repro-toxic	H360		None																																	
Serious environmental implications	H420		None																																	

Fig. S1 Zero pass for *Green Chem.*, 2015, 17, 193–198 (reference 30).



Yield, conversion, selectivity, AE, RME				Summary of Zero Pass Metrics Toolkit													
Reactant (Limiting Reactant First)	Mass (g)	MW	Mol (M)	Catalyst	Mass (PPM)	Reagent	Mass (mg)	Reaction solvent	Volume (cm <sup>3</sup> )	Density (g ml <sup>-1</sup> )	Mass (g)	Work up chemical	Mass (g)	Workup solvent	Volume (cm <sup>3</sup> )	Density (g ml <sup>-1</sup> )	Mass (g)
Glycerol	3.78	92.09	0.04	Ru (CNC)	12.00	KOH	2.30	Water	3.00	1.00	3.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
<b>Total</b>	<b>3.78</b>	<b>92.09</b>			<b>12.00</b>		<b>2.30</b>				<b>3.00</b>		<b>0.00</b>				<b>0.00</b>
										<b>Flag</b>							
$\frac{\text{molecular weight of product}}{\text{total molecular weight of reactants}} \times 100$						Yield	6.8	6.8									
$\frac{\text{mass of isolated product}}{\text{total mass of reactants}} \times 100$						Conversion	100.0	100.0									
						Selectivity	6.8	6.8									
						AE	97.8										
						RME	6.7										
												Product	mass (g)	mw	mol (M)		
													0.252	90.080	0.0027997		
												Unreacted limiting reactant	mass				
<b>Solvents (Zero Pass)</b>				<b>Highly hazardous solvents (Red flag for any of the following)</b>				<b>List Highly Hazardous Solvents Below</b>									
				Et <sub>2</sub> O, Benzene, CCl <sub>4</sub> , chloroform, DCE, nitromethane, CS <sub>2</sub> , HMPA				None									
<b>Health and Safety (Zero Pass)</b>				<b>Health &amp; safety (Red flag for any of the following)</b>				<b>List substances plus the red flagged H-codes below</b>									
				Highly explosive				H200, H201, H202, H203									
				Explosive thermal runaway				H240									
				Fatally toxic				H300, H310, H330									
				Mutagenic				H350									
				Repro-toxic				H360									
				Serious environmental implications				H420									

Fig. S3 Zero pass for *Organometallics* 2018, 37, 1400–1409 (reference 23).



Supplementary Information: Appendix 2				Summary of Zero Pass Metrics Toolkit													
Yield, conversion, selectivity, AE, RME																	
Reactant (Limiting Reactant First)	Mass (mg)	MW	Mol (mM)	Catalyst	Mass ( $\mu\text{mol}$ )	Reagent	Mass (mg)	Reaction solvent	Volume ( $\text{cm}^3$ )	Density ( $\text{g ml}^{-1}$ )	Mass (g)	Work up chemical	Mass (g)	Workup solvent	Volume ( $\text{cm}^3$ )	Density ( $\text{g ml}^{-1}$ )	Mass (g)
Glycerol	236.00	92.09	2.56	Ru (NNN)	0.70	KOH	83.00	EtOH	2.00	0.79	1.58						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
<b>Total</b>	<b>236.00</b>	<b>92.09</b>			<b>0.70</b>		<b>83.00</b>				<b>1.58</b>		<b>0.00</b>				<b>0.00</b>
											<b>Flag</b>						
$\frac{\text{molecular weight of product}}{\text{total molecular weight of reactants}} \times 100$					Yield	90.1	Flag	90.1									
$\frac{\text{mass of isolated product}}{\text{total mass of reactants}} \times 100$					Conversion	100.0	Flag	100.0									
					Selectivity	90.1	Flag	90.1									
					AE	97.8											
					RME	88.1											
												Product	mass (mg)	mw	mol (mM)		
													208.000	90.080	2.3090586		
												Unreacted limiting reactant	mass				
<b>Solvents (Zero Pass)</b>																	
<b>Highly hazardous solvents (Red flag for any of the following)</b>																	
Et <sub>2</sub> O, Benzene, CCl <sub>4</sub> , chloroform, DCE, nitromethane, CS <sub>2</sub> , HMPA							<b>List Highly Hazardous Solvents Below</b>										
							None										
<b>Health and Safety (Zero Pass)</b>																	
<b>Health &amp; safety (Red flag for any of the following)</b>																	
Highly explosive				H200, H201, H202, H203				None									
Explosive thermal runaway				H240				None									
Fatally toxic				H300, H310, H330				None									
Mutagenic				H350				None									
Repro-toxic				H360				None									
Serious environmental implications				H420				None									

**Fig. S5 Zero pass for Chem. Commun., 2020, 56, 9886 (reference 35).**



Supplementary Information: Appendix 2			Summary of Zero Pass Metrics Toolkit																								
Yield, conversion, selectivity, AE, RME																											
Reactant (Limiting Reactant First)	Mass (mg)	MW	Mol (mM)	Catalyst	Mass (mg)	Reagent	Mass (mg)	Reaction solvent	Volume (cm <sup>3</sup> )	Density (g ml <sup>-1</sup> )	Mass (g)	Work up chemical	Mass (g)	Workup solvent	Volume (cm <sup>3</sup> )	Density (g ml <sup>-1</sup> )	Mass (g)										
Glycerol	92.00	92.09	1.00	Ru (NNN)	7.00	KOH	196.00	tBuOH	1.00	0.78	0.78							0.00									
											0.00							0.00									
											0.00							0.00									
											0.00							0.00									
											0.00							0.00									
											0.00							0.00									
											0.00							0.00									
<b>Total</b>	<b>92.00</b>	<b>92.09</b>			<b>7.00</b>		<b>196.00</b>				<b>0.78</b>		<b>0.00</b>					<b>0.00</b>									
$AE = \frac{\text{molecular weight of product}}{\text{total molecular weight of reactants}} \times 100$																											
<table border="0"> <tr> <td>Yield</td> <td>72.2</td> <td>Flag</td> <td>72.2</td> </tr> <tr> <td>Conversion</td> <td>100.0</td> <td></td> <td>100.0</td> </tr> <tr> <td>Selectivity</td> <td>72.2</td> <td></td> <td>72.2</td> </tr> </table>																Yield	72.2	Flag	72.2	Conversion	100.0		100.0	Selectivity	72.2		72.2
Yield	72.2	Flag	72.2																								
Conversion	100.0		100.0																								
Selectivity	72.2		72.2																								
$RME = \frac{\text{mass of isolated product}}{\text{total mass of reactants}} \times 100$																											
<table border="0"> <tr> <td>AE</td> <td>97.8</td> </tr> <tr> <td>RME</td> <td>70.7</td> </tr> </table>																AE	97.8	RME	70.7								
AE	97.8																										
RME	70.7																										
<table border="0"> <tr> <td>Product</td> <td>mass (mg)</td> <td>mw</td> <td>mol (mM)</td> </tr> <tr> <td></td> <td>65,000</td> <td>90,080</td> <td>0.7215938</td> </tr> <tr> <td>Unreacted limiting reactant</td> <td>mass</td> <td></td> <td></td> </tr> </table>																Product	mass (mg)	mw	mol (mM)		65,000	90,080	0.7215938	Unreacted limiting reactant	mass		
Product	mass (mg)	mw	mol (mM)																								
	65,000	90,080	0.7215938																								
Unreacted limiting reactant	mass																										
<b>Solvents (Zero Pass)</b>																											
<b>Highly hazardous solvents (Red flag for any of the following)</b>																											
Et <sub>2</sub> O, Benzene, CCl <sub>4</sub> , chloroform, DCE, nitromethane, CS <sub>2</sub> , HMPA																											
<b>List Highly Hazardous Solvents Below</b>																											
None																											
<b>Health and Safety (Zero Pass)</b>																											
<b>Health &amp; safety (Red flag for any of the following)</b>																											
<b>List substances plus the red flagged H-codes below</b>																											
Highly explosive	H200, H201, H202, H203		None																								
Explosive thermal runaway	H240		None																								
Fatally toxic	H300, H310, H330		None																								
Mutagenic	H350		None																								
Repro-toxic	H360		None																								
Serious environmental implications	H420		None																								

**Fig. S7 Zero pass for RSC Adv., 2024, 14, 37082 (reference 38).**



Supplementary Information: Appendix 2			Summary of Zero Pass Metrics Toolkit																
Yield, conversion, selectivity, AE, RME																			
Reactant (Limiting Reactant First)	Mass (mg)	MW	Mol (mM)	Catalyst	Mass (mg)	Reagent	Mass (mg)	Reaction solvent	Volume (cm <sup>3</sup> )	Density (g ml <sup>-1</sup> )	Mass (g)	Work up chemical	Mass (g)	Workup solvent	Volume (cm <sup>3</sup> )	Density (g ml <sup>-1</sup> )	Mass (g)		
Glycerol	626.00	92.09	6.80	Ru (NN)	7.00	KOH	572.00	water	1.00	1.00	1.00						0.00		
											0.00						0.00		
											0.00						0.00		
											0.00						0.00		
											0.00						0.00		
											0.00						0.00		
											0.00						0.00		
											0.00						0.00		
<b>Total</b>	<b>626.00</b>	<b>92.09</b>			<b>7.00</b>		<b>572.00</b>				<b>1.00</b>		<b>0.00</b>				<b>0.00</b>		
											<b>Flag</b>								
$AE = \frac{\text{molecular weight of product}}{\text{total molecular weight of reactants}} \times 100$											Yield	99.0							
											Conversion	100.0							
											Selectivity	99.0							
$RME = \frac{\text{mass of isolated product}}{\text{total mass of reactants}} \times 100$											AE	97.8							
											RME	96.8							
													Product	mass (mg)	606.000	mw	90.080	mol (mM)	6.7273535
													Unreacted limiting reactant						
<b>Solvents (Zero Pass)</b>																			
<b>Highly hazardous solvents (Red flag for any of the following)</b>																			
Et <sub>2</sub> O, Benzene, CCl <sub>4</sub> , chloroform, DCE, nitromethane, CS <sub>2</sub> , HMPA																			
List Highly Hazardous Solvents Below																			
None																			
<b>Health and Safety (Zero Pass)</b>																			
<b>Health &amp; safety (Red flag for any of the following)</b>																			
List substances plus the red flagged H-codes below																			
Highly explosive																			
H200, H201, H202, H203																			
None																			
Explosive thermal runaway																			
H240																			
None																			
Fatally toxic																			
H300, H310, H330																			
None																			
Mutagenic																			
H350																			
None																			
Repro-toxic																			
H360																			
None																			
Serious environmental implications																			
H420																			
None																			

Fig. S9 Zero pass for *J. Catal.*, 2026, 453, 116442 (reference 42).





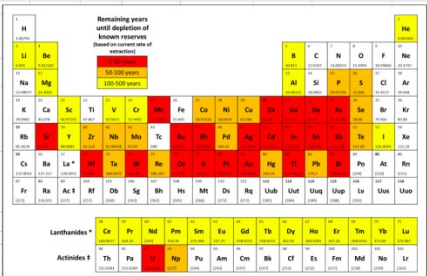
Supplementary Information: Appendix 2				Summary of First Pass Metrics Toolkit															
Yield, AE, RME, M/PMI and OE																			
Reactant (Limiting Reactant First)	Mass (mg)	MW	Mol (mM)	Catalyst	Mass (mg)	Reagent	Mass (mg)	Reaction solvent	Volume (cm <sup>3</sup> )	Density (g ml <sup>-1</sup> )	Mass (g)	Work up chemical	Mass (g)	Workup solvent	Volume (cm <sup>3</sup> )	Density (g ml <sup>-1</sup> )	Mass (g)		
Glycerol	92.00	92.09	1.00	Ru (PP)	33.00	KOH	84.00	EtOH	2.00	0.79	1.58							0.00	
											0.00							0.00	
											0.00							0.00	
											0.00							0.00	
											0.00							0.00	
											0.00							0.00	
											0.00							0.00	
<b>Total</b>	<b>92.00</b>	<b>92.09</b>			<b>33.00</b>		<b>84.00</b>				<b>1.58</b>		<b>0.00</b>					<b>0.00</b>	
											<b>Flag</b>								
											Yield	83.1							
											Conversion	100.0							
											Selectivity	83.1							
											AE	97.8							
											RME	81.9	OE	83.1					
											PMI total	2.8							
											PMI Reaction	2.8							
											PMI reagents, reagents, catalyst	2.8							
											PMI reaction solvents	0.0							
											PMI Workup	0.0							
											PMI Workup chemical	0.0							
											PMI workup solvents	0.0							
											Product	Mass (mg)	MW	Mol (mM)					
												74.770	90.080	0.8300399564					
											Unreacted limiting reagent	mass							
												0.00							
											mass intensity =								
											OE =								
											AE								
											PMI total								
											PMI Reaction								
											PMI reagents, reagents, catalyst								
											PMI reaction solvents								
											PMI Workup								
											PMI Workup chemical								
											PMI workup solvents								
Solvents (First Pass)											List solvents below								
Preferred solvents				water, EtOH, nBuOH, AcOIPr, AcOH, PhOMe, MeOH, tBuOH, BnOH, ethylene glycol, acetone, MEK, MIBK, AcOEt, sulfolane								EtOH							
Problematic solvents: (acceptable only if substitution does not offer advantages)				DMG, cyclohexanone, DMPU, AcOH, Ac <sub>2</sub> O, Acetonitrile, AcOMe, THF, heptane, Me-cyclohexane, toluene, xylene, MTBE, cyclohexane, chlorobenzene, formic acid, pyridine, Me-THF															
Hazardous solvents: These solvents have significant health and/or safety concerns.				dioxane, pentane, TBA, diisopropyl ether, DMG, DCM, DMF, DMA, NMP, methylacetone, hexane															
Highly hazardous solvents: The solvents which are agreed not to be used, even in screening.				Et <sub>2</sub> O, Benzene, CCl <sub>4</sub> , chloroform, DCE, nitromethane, CS <sub>2</sub> , HMPA															
Catalyst/enzyme (First Pass)				Tick		Tick													
Catalyst or enzyme used, or reaction takes place without any catalyst/reagents.				Green Flag	X	Facile recovery of catalyst/enzyme		Green Flag											
Use of stoichiometric quantities of reagents				Amber Flag		catalyst/enzyme not recovered		Amber Flag		X									
Use of reagents in excess				Red Flag															
Critical elements																			
Supply remaining		Flag colour		Note element															
5-50 years		Red Flag		Ru															
50-500 years		Amber Flag																	
>500 years		Green Flag																	
																			
Energy (First Pass)				Tick		Tick													
Reaction run between 0 to 70°C				Green Flag		Reaction run at reflux		Red Flag		X									
Reaction run between -20 to 0 or 70 to 140°C				Amber Flag	X	Reaction run 5°C or more below the solvent boiling point		Green Flag											
Reaction run below -20 or above 140°C				Red Flag															
Batch/flow				Tick		List													
Flow				Green Flag		Work Up													
Batch				Amber Flag		quenching													
						filtration													
						centrifugation													
						crystallisation													
						Low temperature distillation/evaporation/sublimation (< 140 °C at atmospheric pressure)													
						solvent exchange, quenching into aqueous solvent													
						chromatography/ion exchange													
						high temperature multiple recrystallisation													
Health & safety						List substances and H-codes		List substances and H-codes		List substances and H-codes									
Highly explosive				Red Flag		Amber Flag		Green Flag											
				H200, H201, H202, H203		H205, H220, H224		If no red or amber flagged H codes present then green flag											
Explosive thermal runaway				H230, H240, H250		H241													
Toxic				H300, H310, H330		H302, H311, H331													
Long Term toxicity				H340, H350, H360, H370, H372		H341, H351, H361, H371, H373													
Environmental implications				H400, H410, H411, H420		H401, H412													
Use of chemicals of environmental concern						List substances of very high concern													
Chemical identified as Substances of Very High Concern by ChemSec which are utilised				Red Flag															

Fig. S12 First pass for *Catalysts* 2026, 16, 48 (reference 43).

Yield, conversion, selectivity, AE, RME			Summary of Zero Pass Metrics Toolkit															
Reactant (Limiting Reactant First)	Mass (mg)	MW	Mol (mM)	Catalyst	Mass (mol%)	Reagent	Mass (mg)	Reaction solvent	Volume (cm <sup>3</sup> )	Density (g ml <sup>-1</sup> )	Mass (g)	Work up chemical	Mass (g)	Workup solvent	Volume (cm <sup>3</sup> )	Density (g ml <sup>-1</sup> )	Mass (g)	
Glycerol	645.00	92.09	7.00	Ru-1	0.05	NaOH	280.00	Water	0.50	1.00	0.50	CaCO <sub>3</sub>	0.25	Water	5.00	1.00	5.00	
											0.00						0.00	
											0.00						0.00	
											0.00						0.00	
											0.00						0.00	
											0.00						0.00	
											0.00						0.00	
<b>Total</b>	<b>645.00</b>	<b>92.09</b>			<b>0.05</b>		<b>280.00</b>				<b>0.50</b>		<b>0.25</b>				<b>5.00</b>	
										<b>Flag</b>								
$\frac{\text{molecular weight of product}}{\text{total molecular weight of reactants}} \times 100$						Yield	94.0	Flag	94.0									
$\frac{\text{mass of isolated product}}{\text{total mass of reactants}} \times 100$						Conversion	100.0	Flag	100.0									
						Selectivity	94.0	Flag	94.0									
						AE	97.8											
						RME	91.9											
												Product	mass (mg)	593.000	mw	90.080	mol (mM)	6.5830373
												Unreacted limiting reactant	mass					
<b>Solvents (Zero Pass)</b>																		
<b>Highly hazardous solvents (Red flag for any of the following)</b>																		
Et <sub>2</sub> O, Benzene, CCl <sub>4</sub> , chloroform, DCE, nitromethane, CS <sub>2</sub> , HMPA						List Highly Hazardous Solvents Below												
						None												
<b>Health and Safety (Zero Pass)</b>																		
<b>Health &amp; safety (Red flag for any of the following)</b>																		
Highly explosive						H200, H201, H202, H203						List substances plus the red flagged H-codes below						
Explosive thermal runaway						H240						None						
Fatally toxic						H300, H310, H330						None						
Mutagenic						H350						None						
Repro-toxic						H360						None						
Serious environmental implications						H420						None						

Fig. S13 Zero pass for *this work*.



## 1.2 E-factor calculations

**E-factor for *Green Chem.*, 2015, 17, 193–198 (reference 30)**

$$\text{E-factor} = [12.6 \text{ g (Gly)} + 8.24 \text{ g (NMP)} + 0.00000579 \text{ g (Ru cat.)} + 5.92 \text{ g (NaOH)} - 8.264 \text{ g (Product LA)}] / 8.264 \text{ g (Product LA)} = \mathbf{2.2}$$

**E-factor for *Organometallics* 2018, 37, 1400–1409 198 (reference 23)**

$$\text{E-factor} = [3.78 \text{ g (Gly)} + 3 \text{ g (H}_2\text{O)} + 0.0036 \text{ g (Ru cat.)} + 2.36 \text{ g (KOH)} - 0.258 \text{ g (Product LA)}] / 0.258 \text{ g (Product LA)} = \mathbf{34.4}$$

**E-factor for *Chem. Commun.*, 2020, 56, 9886 198 (reference 35)**

$$\text{E-factor} = [0.235 \text{ g (Gly)} + 1.578 \text{ g (EtOH)} + 0.0007 \text{ g (Ru cat.)} + 0.083 \text{ g (KOH)} - 0.204 \text{ g (Product LA)}] / 0.204 \text{ g (Product LA)} = \mathbf{8.3}$$

**E-factor for *RSC Adv.*, 2024, 14, 37082 (reference 38)**

$$\text{E-factor} = [0.092 \text{ g (Gly)} + 0.078 \text{ g (tBuOH)} + 0.007 \text{ g (Ru cat.)} + 0.196 \text{ g (KOH)} - 0.065 \text{ g (Product LA)}] / 0.065 \text{ g (Product LA)} = \mathbf{4.7}$$

**E-factor for *J. Catal.*, 2026, 453, 116442 (reference 42)**

$$\text{E-factor} = [0.626 \text{ g (Gly)} + 1.0 \text{ g (H}_2\text{O)} + 0.007 \text{ g (Ru-1)} + 0.572 \text{ g (KOH)} - 0.606 \text{ g (Product LA)}] / 0.606 \text{ g (Product LA)} = \mathbf{2.6}$$

**E-factor for *Catalysts* 2026, 16, 48 (reference 43)**

$$\text{E-factor} = [0.092 \text{ g (Gly)} + 2.53 \text{ g (EtOH)} + 0.032 \text{ g (Ru-1)} + 0.084 \text{ g (KOH)} - 0.075 \text{ g (Product LA)}] / 0.075 \text{ g (Product LA)} = \mathbf{35.5}$$

**E-factor for this work**

$$\text{E-factor} = [0.6426 \text{ g (Gly)} + 0.51 \text{ g (H}_2\text{O)} + 0.0025 \text{ g (Ru-1)} + 0.280 \text{ g (NaOH)} - 0.593 \text{ g (Product LA)}] / 0.593 \text{ g (Product LA)} = \mathbf{1.4}$$

**E-factor for gram-scale reactions**

$$\text{E-factor} = [3.276 \text{ g (Gly)} + 2.45 \text{ g (H}_2\text{O)} + 0.0125 \text{ g (Ru-1)} + 1.4 \text{ g (NaOH)} - 2.964 \text{ g (Product LA)}] / 2.964 \text{ g (Product LA)} = \mathbf{1.4}$$

$$\text{E-factor} = [6.426 \text{ g (Gly)} + 4.9 \text{ g (H}_2\text{O)} + 0.025 \text{ g (Ru-1)} + 2.8 \text{ g (NaOH)} - 5.801 \text{ g (Product LA)}] / 5.801 \text{ g (Product LA)} = \mathbf{1.4}$$

$$\text{E-factor} = [12.852 \text{ g (Gly)} + 9.8 \text{ g (H}_2\text{O)} + 0.05 \text{ g (Ru-1)} + 5.6 \text{ g (NaOH)} - 11.728 \text{ g (Product LA)}] / 11.728 \text{ g (Product LA)} = \mathbf{1.4}$$

$$\text{E-factor} = [6.426 \text{ g (Gly)} + 4.9 \text{ g (H}_2\text{O)} + 0.01 \text{ g (Ru-1)} + 2.8 \text{ g (NaOH)} - 5.685 \text{ g (Product LA)}] / 5.685 \text{ g (Product LA)} = \mathbf{1.5}$$

$$\text{E-factor} = [12.852 \text{ g (Gly)} + 9.8 \text{ g (H}_2\text{O)} + 0.02 \text{ g (Ru-1)} + 5.6 \text{ g (NaOH)} - 9.988 \text{ g (Product LA)}] / 9.988 \text{ g (Product LA)} = \mathbf{1.8}$$

$$\text{E-factor} = [19.278 \text{ g (Gly)} + 14.7 \text{ g (H}_2\text{O)} + 0.03 \text{ g (Ru-1)} + 8.4 \text{ g (NaOH)} - 14.983 \text{ g (Product LA)}] / 14.983 \text{ g (Product LA)} = \mathbf{1.8}$$

$$\text{E-factor} = [25.704 \text{ g (Gly)} + 19.6 \text{ g (H}_2\text{O)} + 0.04 \text{ g (Ru-1)} + 11.2 \text{ g (NaOH)} - 19.509 \text{ g (Product LA)}] / 19.509 \text{ g (Product LA)} = \mathbf{1.9}$$

### 1.3 EcoScale analysis

Reagents										
Link										
	identifier*	name	MF*	MW	density	purity*	ml	g	mmoles	equiv.
1	[Name, MF or RN]	Glycerol	C3H8O3	92.09	1.26	100%	10	12.6	136.82267347	1
2		Water	H2O	18	1	100%	2.5	2.5	138.88888888	1.0151014109
3		Sodium hydroxide	NaOH	39.997		100%	0	5.914	147.86108958	1.0806768047
4		N-Methyl-2-Pyrrolidone	C5H9NO	99.13	1.028	100%	8	8.224	82.961767376	0.6063451712
5		Ru-MACHO	C29H30NP2RuC	607.0125		100%	0	0.000006	0.0000095385	6.9714458300

Products										
identifier*	name	MF*	MW	g	mmoles	g theor	yield			
	Lactic acid	C3H3O3	90.08	8.264	91.740674955	12.324986	67.0508			

Conditions										
Reagents	Name	mmoles	eq.	Bp	Hazard	Price				
	Glycerol	16.55	1							
	Water	16.8	1.01							
	Sodium hydroxide	17.89	1.08							
	N-Methyl-2-Pyrrolidone	10.03	0.6							
	Ru-MACHO	0	0							
Yield						67				
Price / availability							-16			
Safety							-25			
							0			
Technical setup	Possible items		Selected items							
	Common set-up		(inert) gas atmosphere							
	Instruments for controlled addition of chemicals		Common set-up							
	Unconventional activation technique									
Temperature / time	Possible items		Selected items							
	Heating, > 1h		Heating, > 1h							
	Cooling to 0°C									
	Cooling, < 0°C									
Workup and purification	Possible items		Selected items							
	None		Cooling to room temperature							
	Cooling to room temperature									
	Adding solvent									
EcoScale							55			

Fig. S15 EcoScale analysis for *Green Chem.*, 2015, 17, 193–198 (reference 30).

Reagents										
Link										
	identifier*	name	MF*	MW	density	purity*	ml	g	mmoles	equiv.
1	[Name, MF or RN]	Glycerol	C3H8O3	92.09	1.26	100%	3	3.78	41.046802041	1
2		Water	H2O	18	1	100%	3	3	166.66666666	4.0604056437
3		Potassium hydroxide	KOH	56.10		100%	0	2.36	42.067736185	1.0248724405
4		Ru	C27H33N5O6S2	724.2311		100%	0	0.00036	0.0004970789	0.0000121100

Products										
identifier*	name	MF*	MW	g	mmoles	g theor	yield			
	Lactic acid	C3H3O3	90.08	0.258	2.8641207815	3.697496	6.9777000000			

Conditions										
Reagents	Name	mmoles	eq.	Bp	Hazard	Price				
	Glycerol	159.09	1							
	Water	645.99	4.06							
	Potassium hydroxide	163.05	1.02							
	Ru	0	0							
Yield						7				
Price / availability							-47			
Safety							-20			
							0			
Technical setup	Possible items		Selected items							
	Common set-up		Common set-up							
	Instruments for controlled addition of chemicals		Instruments for controlled addition of chemicals							
	Unconventional activation technique									
Temperature / time	Possible items		Selected items							
	Heating, > 1h		Heating, > 1h							
	Cooling to 0°C									
	Cooling, < 0°C									
Workup and purification	Possible items		Selected items							
	Sublimation		Cooling to room temperature							
	Liquid - liquid extraction or washing									
	Classical chromatography									
EcoScale							29			

Fig. S16 EcoScale analysis for *Organometallics* 2018, 37, 1400–1409 (reference 23).

Reagents										
Link										
	identifier*	name	MF*	MW	density	purity*	ml	g	mmoles	equiv.
1	Name, MF or RN	Glycerol	C3H8O3	92.09	1.26	100%	0.186508	0.235	2.5518514496	1
2		Potassium hydroxide	KOH	56.1056		100%	0	0.083	1.4793532196	0.5797176084
3		Ethanol	C2H6O	46.068	0.789	100%	2	1.578	34.253711904	13.423082252
4		Ru	C55H43N5RuP2	1007.9		100%	0	0.0007	0.0006945133	0.0002721605

Products										
identifier*	name	MF*	MW	g	mmoles	g theor.	yield:			
	Lactic acid	C3H3O3	90.08	0.204	2.2646536412	0.229871	88.745399999			

Conditions										
Reagents	Name	mmoles	eq.	Bp	Hazard	Price				
	Glycerol	12.5	1							
	Potassium hydroxide	7.25	0.57							
	Ethanol	167.91	13.42							
	Ru	0	0							
Yield						89				
Price / availability							-6			
Safety							-20			
Technical setup	Possible items					Selected items				
	Any additional special glassware					Common set-up				
	(Inert) gas atmosphere					(Inert) gas atmosphere				
	Glove box									
Temperature / time	Possible items					Selected items				
	Heating, > 1h					Heating, > 1h				
	Cooling to 0°C									
	Cooling, < 0°C									
Workup and purification	Possible items					Selected items				
	Simple filtration					Cooling to room temperature				
	Removal of solvent with bp < 150°C									
	Countertop, and filtration									
EcoScale							70			

Fig. S17 EcoScale analysis for *Chem. Commun.*, 2020, 56, 9886 (reference 35).

Reagents										
Link										
	identifier*	name	MF*	MW	density	purity*	ml	g	mmoles	equiv.
1	Name, MF or RN	Glycerol	C3H8O3	92.09	1.26	100%	0.073016	0.092	0.9990226951	1
2		tert-Butyl alcohol	C4H10O	74.12	0.781	100%	1	0.781	10.536967080	10.547274982
3		Potassium Hydroxide	KOH	56.1056		100%	0	0.196	3.4934124222	3.4968298909
4		Ru(NNN)	C31H30N3O2Cl	679.5438		100%	0	0.007	0.0103010284	0.0103111055

Products										
identifier*	name	MF*	MW	g	mmoles	g theor.	yield:			
	Lactic acid	C3H3O3	90.08	0.065	0.7215808170	0.089992	72.2286			

Conditions										
Reagents	Name	mmoles	eq.	Bp	Hazard	Price				
	Glycerol	15.36	1							
	tert-Butyl alcohol	162.1	10.54							
	Potassium Hydroxide	53.74	3.49							
	Ru(NNN)	0.15	0.01							
Yield						72				
Price / availability							-14			
Safety							-20			
Technical setup	Possible items					Selected items				
	Any additional special glassware					Common set-up				
	(Inert) gas atmosphere					(Inert) gas atmosphere				
	Glove box									
Temperature / time	Possible items					Selected items				
	Heating, > 1h					Heating, > 1h				
	Cooling to 0°C									
	Cooling, < 0°C									
Workup and purification	Possible items					Selected items				
	None					Adding solvent				
	Cooling to room temperature					Cooling to room temperature				
	Adding solvent									
EcoScale							62			

Fig. S18 EcoScale analysis for *RSC Adv.*, 2024, 14, 37082 (reference 38).

Reagents										
Link										
	identifier*	name	MF*	MW	density	purity*	ml	g	mmoles	equiv.
1	<input type="text" value="Name, MF or RN"/>	Glycerol	C3H8O3	92.09	1.26	100%	0.496825	0.626	6.7976979042	1
2	<input type="text"/>	Water	H2O	18	1	100%	1	1	55.5555555555	8.1727014554
3	<input type="text"/>	Potassium Hydroxide	KOH	56.1056		100%	0	0.572	10.195060742	1.4997813798
4	<input type="text"/>	Ru(NN)	C22H23N3OCl2I	517.416		100%	0	0.007	0.0135287660	0.0019901981

Products										
identifier*	name	MF*	MW	g	mmoles	g theor	yield			
<input type="text"/>	Lactic acid	C3H3O3	90.08	0.606	6.7273534635	0.612337	98.965099999			

Conditions										
Reagents	Name	mmoles	eq.	Bp	Hazard	Price				
	Glycerol	11.21	1							
	Water	91.67	8.17							
	Potassium Hydroxide	16.82	1.49							
	Ru(NN)	0.02	0							
Yield	<input type="text" value="99"/>					<input type="text" value="-1"/>				
Price / availability						<input type="text" value="-20"/>				
Safety						<input type="text" value="0"/>				
Technical setup	Possible items Any additional special glassware (inert) gas atmosphere Glove box		Selected items Common set-up			<input type="text" value="0"/>				
Temperature / time	Possible items Heating, > 1h Cooling to 0°C Cooling, < 0°C		Selected items Heating, > 1h			<input type="text" value="-3"/>				
Workup and purification	Possible items None Cooling to room temperature Adding solvent		Selected items Adding solvent Cooling to room temperature			<input type="text" value="0"/>				
EcoScale						<input type="text" value="76"/>				

Fig. S19 EcoScale analysis for *J. Catal.*, 2026, 453, 116442 (reference 42).

Reagents										
Link										
	identifier*	name	MF*	MW	density	purity*	ml	g	mmoles	equiv.
1	<input type="text" value="Name, MF or RN"/>	Glycerol	C3H8O3	92.09	1.26	100%	0.073016	0.092	0.9990226951	1
2	<input type="text"/>	Ethanol	C2H6O	46.07	0.789	100%	2	1.578	34.252224875	34.285732486
3	<input type="text"/>	Potassium hydroxide	KOH	56.1056		100%	0	0.086	1.5328238179	1.5343233195
4	<input type="text"/>	Ru(PP)	C35H48N3P3Ru	658		100%	0	0.032	0.0486322188	0.0486797938

Products										
identifier*	name	MF*	MW	g	mmoles	g theor	yield			
<input type="text"/>	Lactic acid	C3H3O3	90.08	0.075	0.8325932504	0.089992	83.3407			

Conditions										
Reagents	Name	mmoles	eq.	Bp	Hazard	Price				
	Glycerol	13.32	1							
	Ethanol	456.69	34.28							
	Potassium hydroxide	20.43	1.53							
	Ru(PP)	0.64	0.04							
Yield	<input type="text" value="83"/>					<input type="text" value="-8"/>				
Price / availability						<input type="text" value="-20"/>				
Safety						<input type="text" value="0"/>				
Technical setup	Possible items Instruments for controlled addition of chemicals Unconventional activation technique Pressure equipment, > 1 atm		Selected items Common set-up			<input type="text" value="0"/>				
Temperature / time	Possible items Heating, > 1h Cooling to 0°C Cooling, < 0°C		Selected items Heating, < 1h			<input type="text" value="-2"/>				
Workup and purification	Possible items None Cooling to room temperature Adding solvent		Selected items Cooling to room temperature			<input type="text" value="0"/>				
EcoScale						<input type="text" value="70"/>				

Fig. S20 EcoScale analysis for *Catalysts* 2026, 16, 48 (reference 43).

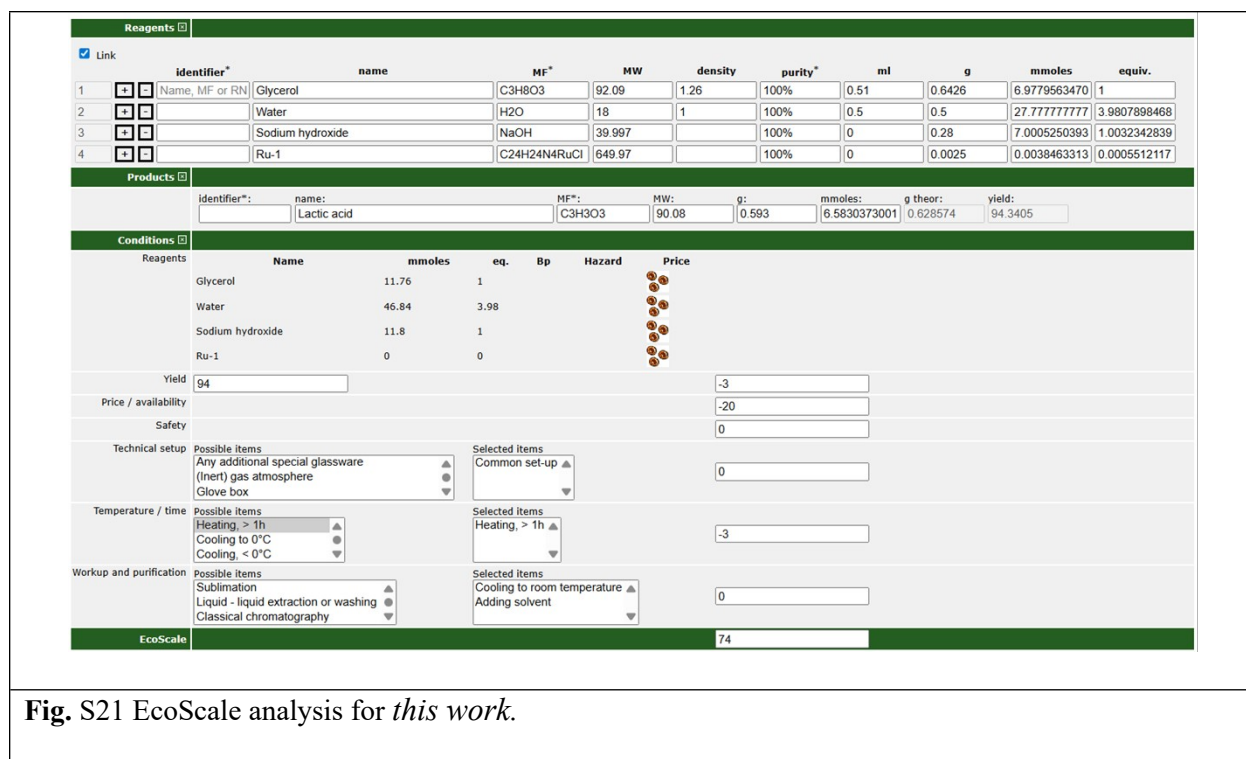


Fig. S21 EcoScale analysis for *this work*.

## 1.4 Calculation of catalyst price

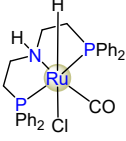
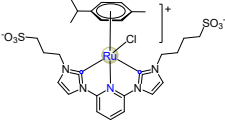
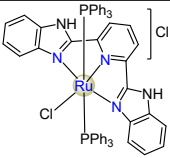
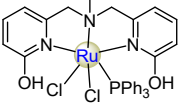
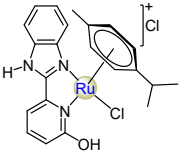
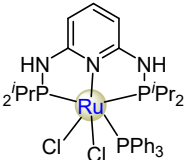
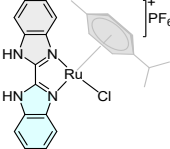
Table S1. Price calculation of ruthenium reported catalysts and our catalyst.				
Chemicals	Company	Price per gram or mL	Required amount (g or mL)	Price for the required amount in INR
<b>Ru-MACHO catalyst by Beller et. al (<i>Green Chem.</i>, 2015, 17, 193–198) (reference 30).</b>				
<b>Ru-MACHO [RuHCl(PNP<sup>Ph</sup>)CO]</b>	Sigma-Aldrich	Price per gram = 15,400/-		
<b>Ru catalyst Voutchkova-Kostal et al. (<i>Organometallics</i> 2018, 37, 1400–1409) (reference 23).</b>				
<b>Ligand</b>	3,3'-(pyridine-2,6-diylbis(1H-imidazole-2,1-diyl))bis(propane-1-sulfonate)			
Step 1	2,6-di(1H-imidazol-2-yl)pyridine			
2,6-Pyridinedicarbonitrile	Sigma-Aldrich	6160/-	0.710	4,374/-
MeOH	SRL Chem.	0.2/-	15	3/-
Aminoacetaldehyde diethyl acetal	Sigma-Aldrich	95.80/-	4.5	431.10/-
Acetic acid	Sigma-Aldrich	5.4/-	2.1	11.32/-
NaOMe	Sigma-Aldrich	2.92/-	2.4	7/-
Price for (Yield = 2.7 g)				4,826.42/-
Price per gram in INR				1,787.56/-
Step 2	3,3'-(pyridine-2,6-diylbis(1H-imidazole-2,1-diyl))bis(propane-1-sulfonate)			

2,6-di(1H-imidazol-2-yl)pyridine	From step 1	1,787.56/-	1.352	2,417/-
1,3-propanesultone	Sigma-Aldrich	145.27/-	3.14	456/-
KOH	SRL Chem.	0.85/-	1.44	1/-
nBu4NBr	Sigma-Aldrich	54.45/-	0.14	8/-
DMSO	SRL Chem.	1.92/-	10	19/-
Price for (Yield = 2.1 g)				2,901/-
Price per gram in INR				1,381.43/-
<b>Metal Precursor</b>	[Ru(p-cymene)Cl <sub>2</sub> ] <sub>2</sub>	Price per gram in INR = 9,250/-		
<b>Ru-Complex</b>				
3,3'-(pyridine-2,6-diylbis(1H-imidazole-2,1-diyl))bis(propane-1-sulfonate)	From step 2	1,381.43/-	0.024	33/-
[Ru(p-cymene)Cl <sub>2</sub> ] <sub>2</sub>	Sigma-Aldrich	9,250/-	0.098	907/-
Ag <sub>2</sub> O	Sigma-Aldrich	1,606/-	0.063	101/-
NaCl	SRL Chem.	0.4/-	0.016	0/-
MeOH	SRL Chem.	0.2/-	16	3/-
Price for (Yield = 0.046 g)				1,044/-
Price per gram of Ru-Complex in INR				22,759/-
<b>Ru catalyst Kumar et al.</b> ( <i>Chem. Commun.</i> , 2020, 56, 9886) (reference 35).				
<b>Ligand</b>	2,6-bis(1H-benzimidazol-2-yl)pyridine			
pyridene-2,6-dicarboxylic acid	Sigma-Aldrich	195.8/-	0.100	20/-
o-penylenediamine	Sigma-Aldrich	51.53/-	0.130	7/-
orthophosphoric acid	Sigma-Aldrich	45.68/-	10	457/-
Price for (Yield = 0.135 g)				484/-
Price per gram in INR				3,586.44/-
<b>Complex</b>				
RuCl <sub>2</sub> (PPh <sub>3</sub> ) <sub>3</sub>	Sigma-Aldrich	3,930/-	0.07	983/-
2,6-Bis(2-benzimidazolyl)pyridine	From above	3,586.44/-	0.250	251/-
THF	SRL Chem.	0.54/-	5	7/-
Price for (Yield = 0.135 g)				1,241/-
Price of Ru-complex per gram in INR				9,146/-
<b>Ru catalyst Daw et al.</b> ( <i>RSC Adv.</i> , 2024, 14, 37082) (reference 38).				
<b>Ligand</b>	6,6'-((methylazanediy)bis(methylene))bis(pyridin-2-ol)			
Step 1	2-methoxy-6-methylpyridine			
2-Bromo-6-methylpyridine	Sigma-Aldrich	1,510/-	5	7,550/-
sodium methoxide	Sigma-Aldrich	11.48/-	6.28	72.1/-
MeOH	SRL Chem.	0.2/-	20	4/-
Price for (Yield = 3.18 g)				7,626.1/-
Price per gram in INR				2,398.14/-
Step 2	(6-methoxypyridin-2-yl)methanol			
6,6'-((methylazanediy)bis(	From above	2,398.14/-	3	7,194.42/-

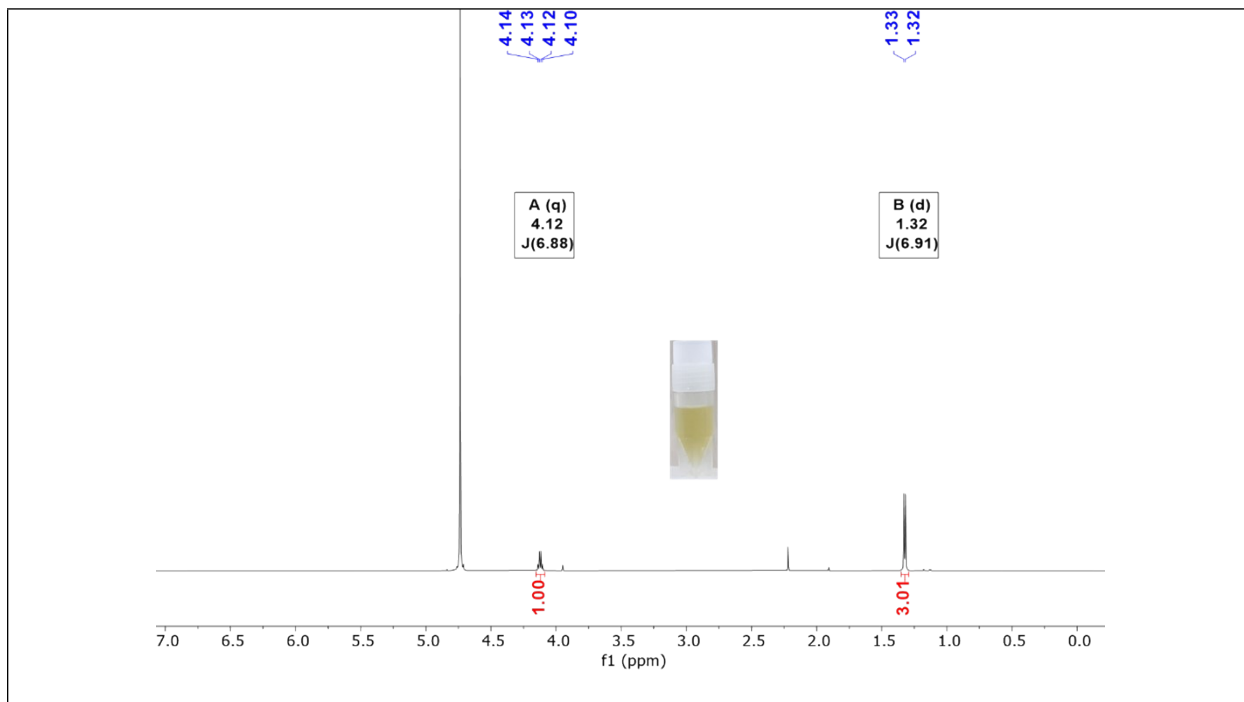
methylene))bis(pyridin-2-ol)				
m-Chloroperbenzoic acid	Sigma-Aldrich	44.5/-	3.56	158.42/-
CHCl <sub>3</sub>	SRL Chem.	3/-	25	75/-
acetic anhydride	TCI	15/-	5	75/-
MeOH	SRL Chem.	0.2/-	10	2/-
KOH	SRL Chem.	1/-	2.7	2.7/-
Price for (Yield = 2.47 g)				7,507.54/-
Price per gram in INR				3,039.5/-
Step 3	1-(6-methoxypyridin-2-yl)-N-((6-methoxypyridin-2-yl)methyl)-N-methylmethanamine			
(6-methoxypyridin-2-yl)methanol	From above	3,039.5/-	2	6,079/-
DCM	SRL Chem.	2.9/-	15	43.5/-
thionyl chloride	Sigma-Aldrich	7.7/-	5.4	41.6/-
methylamine	Sigma-Aldrich	57/-	6	342/-
NaOH	SRL Chem.	0.42/-	4.26	1.8/-
Price for (Yield = 1.7 g)				6,507/-
Price per gram in INR				3,827.6/-
Step 4	6,6'-((methylazanediyl)bis(methylene))bis(pyridin-2-ol)			
1-(6-methoxypyridin-2-yl)-N-((6-methoxypyridin-2-yl)methyl)-N-methylmethanamine	From above	3,827.6/-	1.5	5,741.4/-
Hydrobromic acid	Sigma-Aldrich	9.7/-	2	19.4/-
Acetic acid	SRL Chem.	0.84	2	1.7/-
Price for (Yield = 1.0 g)				5,762.5/-
Price per gram in INR				5,762.5/-
Complex				
RuCl <sub>2</sub> (PPh <sub>3</sub> ) <sub>3</sub>	Sigma-Aldrich	3,930/-	0.390	1,532.7/-
6,6'-((methylazanediyl)bis(methylene))bis(pyridin-2-ol)	From above	5,762.5/-	0.1	576.25/-
Price for (Yield = 0.2 g)				2,109/-
Price of Ru-complex per gram in INR				10,545/-
<b>Ru catalyst Feng Li et al. (<i>J. Catal.</i>, 2026, 453, 116442) (reference 42).</b>				
Ligand	6-(1H-benzo[d]imidazol-2-yl)pyridin-2-ol			
<i>o</i> -phenylenediamine	Sigma-Aldrich	14/-	0.540	7.56/-
6-hydroxypicolinic acid	Sigma-Aldrich	439.5/-	0.835	367/-
polyphosphoric acid	SRL Chem.	1.6/-	25	40/-
Price for (Yield = 0.908 g)				414.56/-
Price per gram in INR				457/-
<b>Metal Precursor</b>	[Ru(p-cymene)Cl <sub>2</sub> ] <sub>2</sub>		Price per gram in INR = 9,250/-	
[Ru(p-cymene)Cl <sub>2</sub> ] <sub>2</sub>	Sigma-Aldrich	9,250/-	0.100	925/-
6-(1H-benzo[d]imidazol-2-	From above	457/-	0.76	347.32/-

yl)pyridin-2-ol				
THF	SRL Chem.	0.54/-	5	2.7/-
Price for (Yield = 0.127 g)				1,275/-
Price of Ru-complex per gram in INR				10,040/-
<b>Ru catalyst Gonsalvi et al. (<i>Catalysts</i> 2026, 16, 48) (reference 43).</b>				
<b>Ligand</b>	N <sup>2</sup> ,N <sup>6</sup> -bis(diisopropylphosphaneyl)pyridine-2,6-diamine			
2,6-Diaminopyridine	Sigma-Aldrich	100.82/-	0.109	11/-
Diisopropylchlorophosphine	Sigma-Aldrich	1418/-	0.38	538.84/-
Triethylamine	SRL Chem.	0.54/-	0.35	0.189/-
THF	SRL Chem.	0.54/-	15	8.1
Price for (Yield = 0.240 g)				558.13/-
Price per gram in INR				2327.4/-
<b>Catalyst</b>				
RuCl <sub>2</sub> (PPh <sub>3</sub> ) <sub>3</sub>	Sigma-Aldrich	3,930/-	0.390	1,532.7/-
N <sup>2</sup> ,N <sup>6</sup> -bis(diisopropylphosphaneyl)pyridine-2,6-diamine	From above		0.1	232.74/-
Price for (Yield = 0.120 g)				1765.44/-
Price of Ru-complex per gram in INR				14,723.77/-
<b>Ru(II)-paracymene catalysts (This Work)</b>				
<b>Ligand</b>	Bis-benzimidazole			
O-phenylenediamine	Sigma-Aldrich	14/-	13.6	190/-
Orthophosphoric acid	Sigma-Aldrich	4.5/-	50	225/-
Trichloroacetic acid	Sigma-Aldrich	26/-	16.3	424/-
Price for (Yield = 11.8 g)				839/-
Price per gram in INR				70/-
<b>Metal Precursor</b>	[Ru(p-cym)Cl <sub>2</sub> ] <sub>2</sub>			
RuCl <sub>3</sub>	Sigma-Aldrich	1944/-	2	3888/-
α-phelandrene	Sigma-Aldrich	14/-	5	70/-
MeOH	SRL Chem.	0.2/-	20	4/-
Price for (Yield = 2 g)				3962/-
Price per gram in INR				1981/-
<b>Ru(II)P-cym complex</b>				
[Ru(p-cym)Cl <sub>2</sub> ] <sub>2</sub>	From above	1981/-	0.153	303/-
Bis-benzimidazole	From above	70/-	0.117	8.19/-
KPF <sub>6</sub>	Sigma-Aldrich	5/-	0.184	0.92/-
MeOH		0.2/-	20	4/-
Price for (Yield = 0.230 g)				316.11/-
Price of Ru(II)P-cym complex per gram in INR				1374.38/-

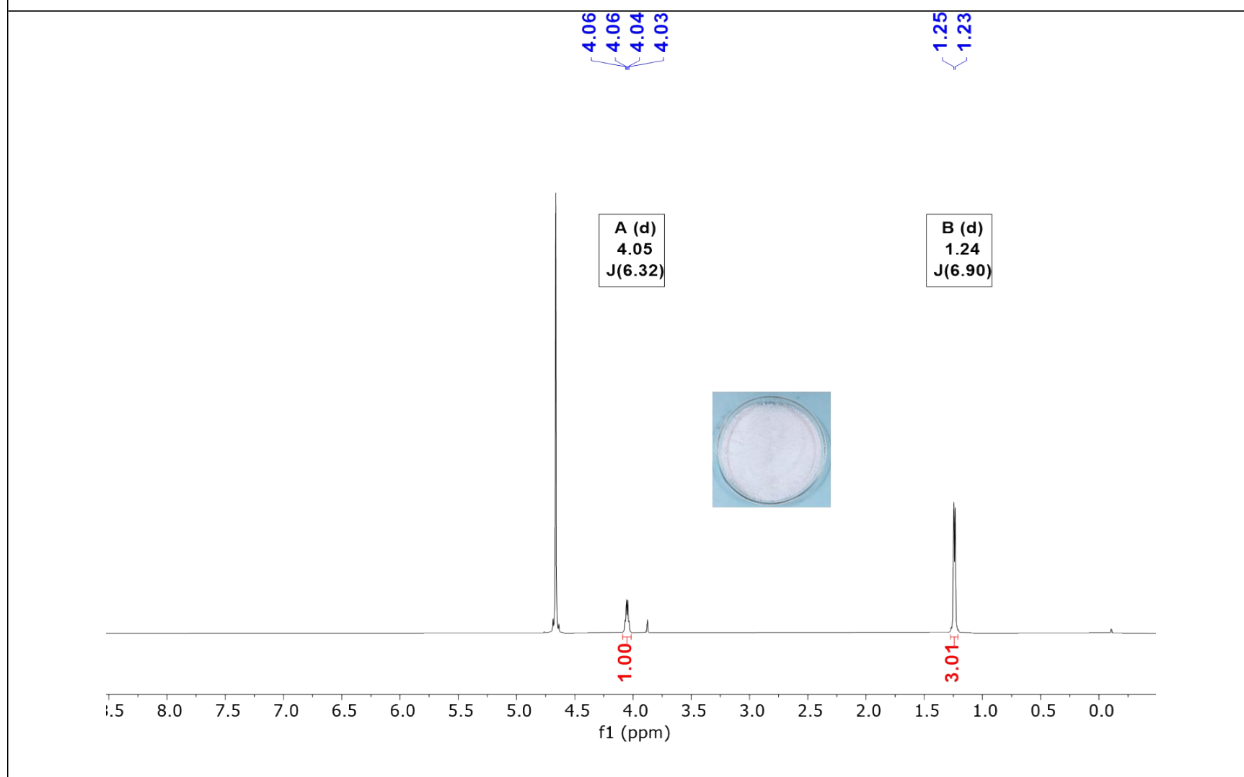
**Table S2.** Price comparison of our catalyst with reported ruthenium catalysts.

Complex	Reference No.	Catalyst Price per gram in INR (₹)	Catalyst Price per gram in US dollars (\$)	Reported catalysts cost comparison with our catalysts per time
	30	15,400/-	175	11.2
	23	22,759/-	258.62	16.6
	35	9,196/-	104.5	6.7
	38	10,545/-	120	7.7
	42	10,040/-	114	7.3
	43	14,723.77/-	156.22	10
	This Work	1,375/-	15.62	1

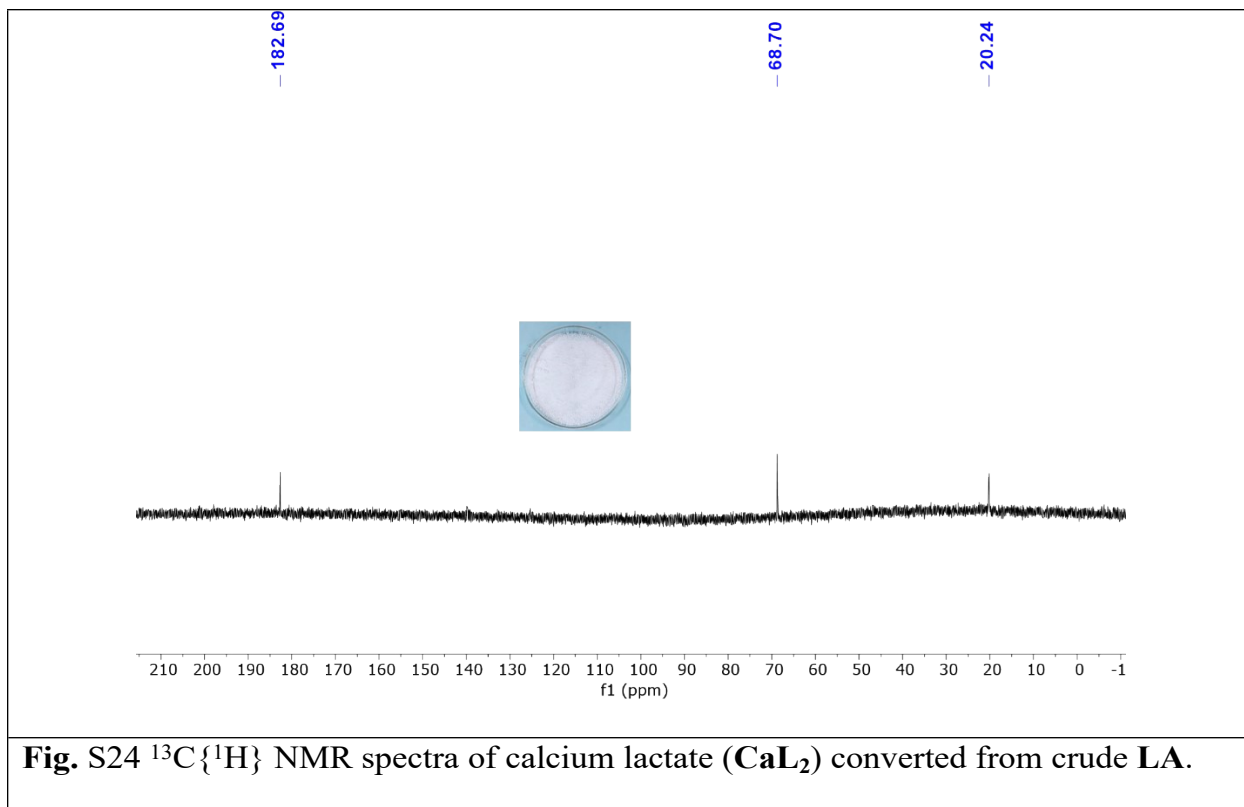
## 1.5 Isolation of crude lactic acid and calcium lactate



**Fig. S22**  $^1\text{H}$  NMR spectra of isolated crude **LA** from the reaction mixture.



**Fig. S23**  $^1\text{H}$  NMR spectra of calcium lactate ( $\text{CaL}_2$ ) converted from crude **LA**.



## 2. $^1\text{H}$ and $^{13}\text{C}$ spectra of ligand (L-5 to L-10) and Complexes (Ru-5 to Ru-10)

### 2.1 $^1\text{H}$ and $^{13}\text{C}$ NMR spectra of ligand (L-5 to L-10)

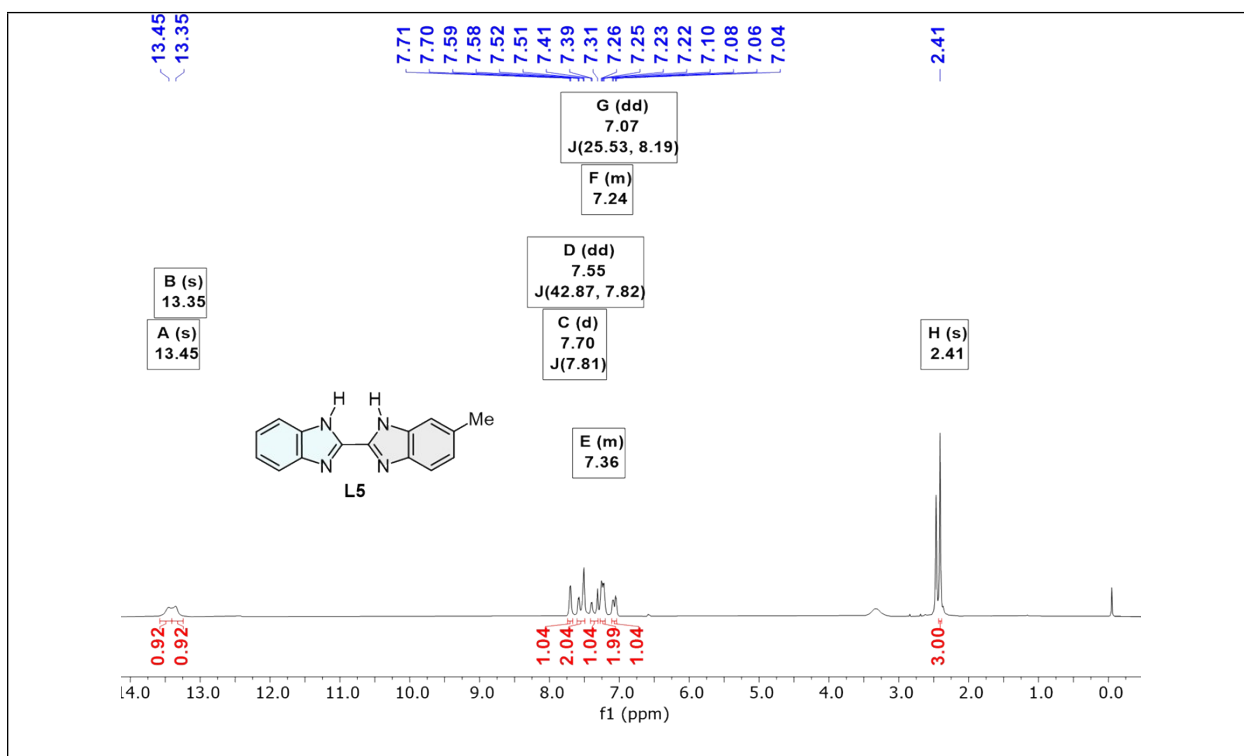
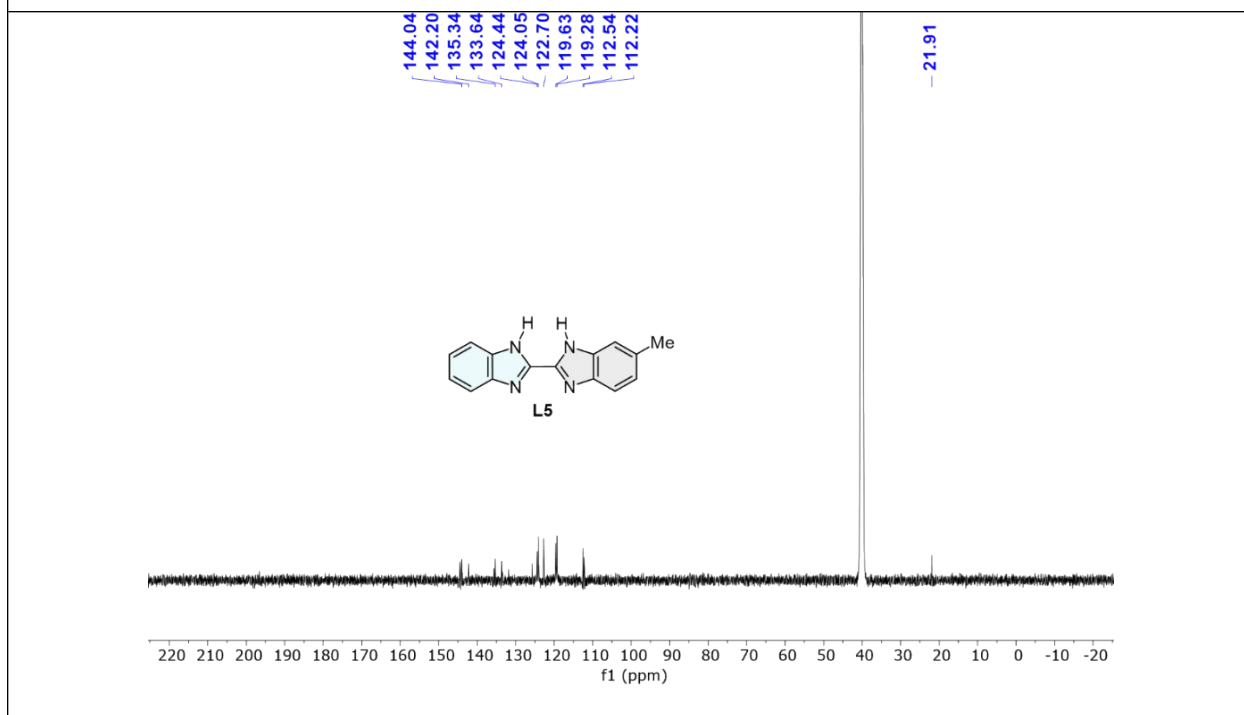
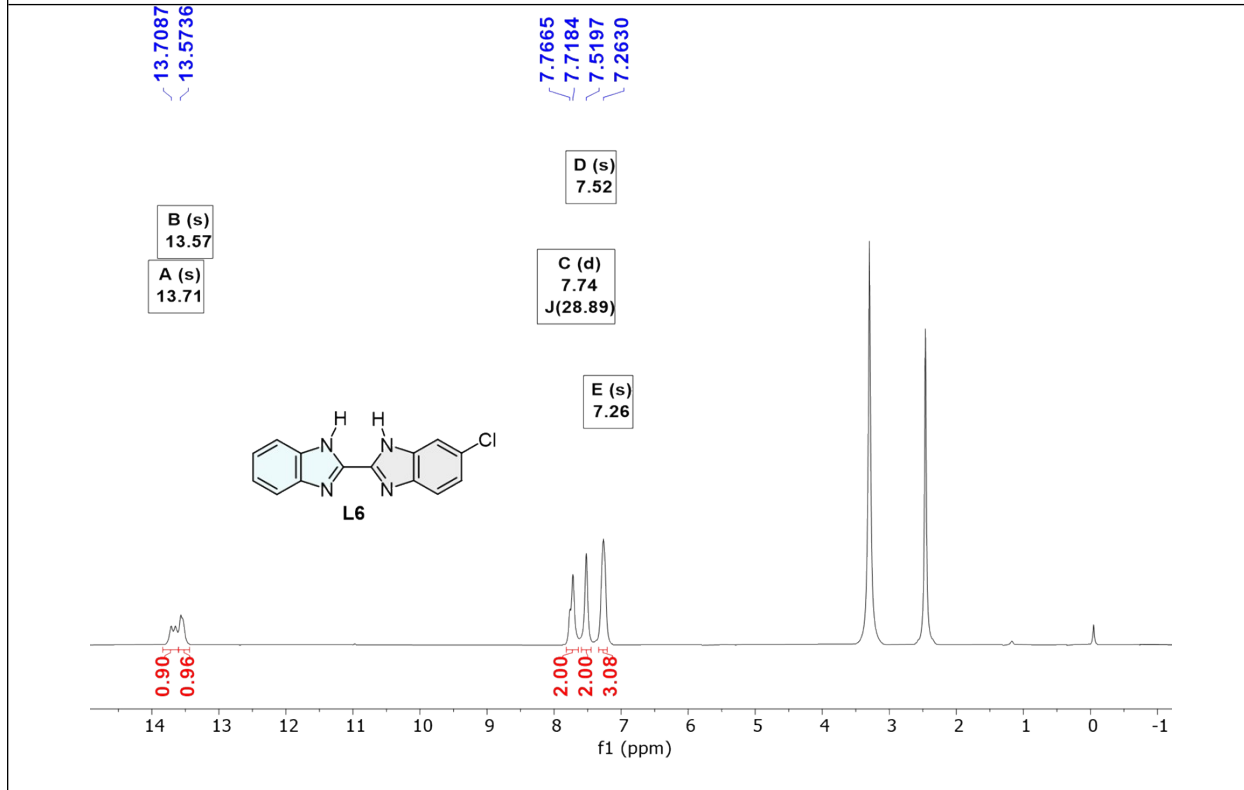


Fig. S25  $^1\text{H}$  NMR spectra of L-5 in DMSO- $d_6$  at 298K.



**Fig. S26**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectra of **L-5** in  $\text{DMSO-d}_6$  at 298K.



**Fig. S27**  $^1\text{H}$  NMR spectra of **L-6** in  $\text{DMSO-d}_6$  at 298K.

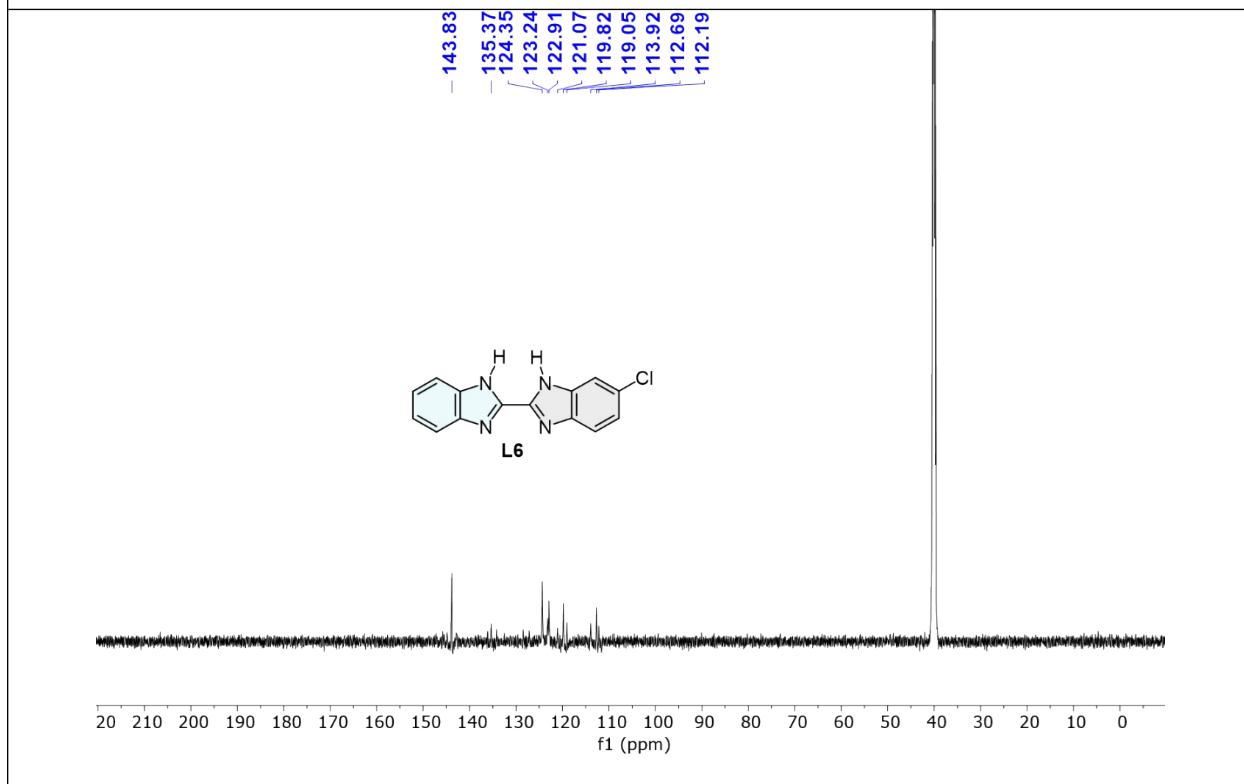


Fig. S28  $^{13}\text{C}\{^1\text{H}\}$  NMR spectra of L-6 in DMSO- $d_6$  at 298K.

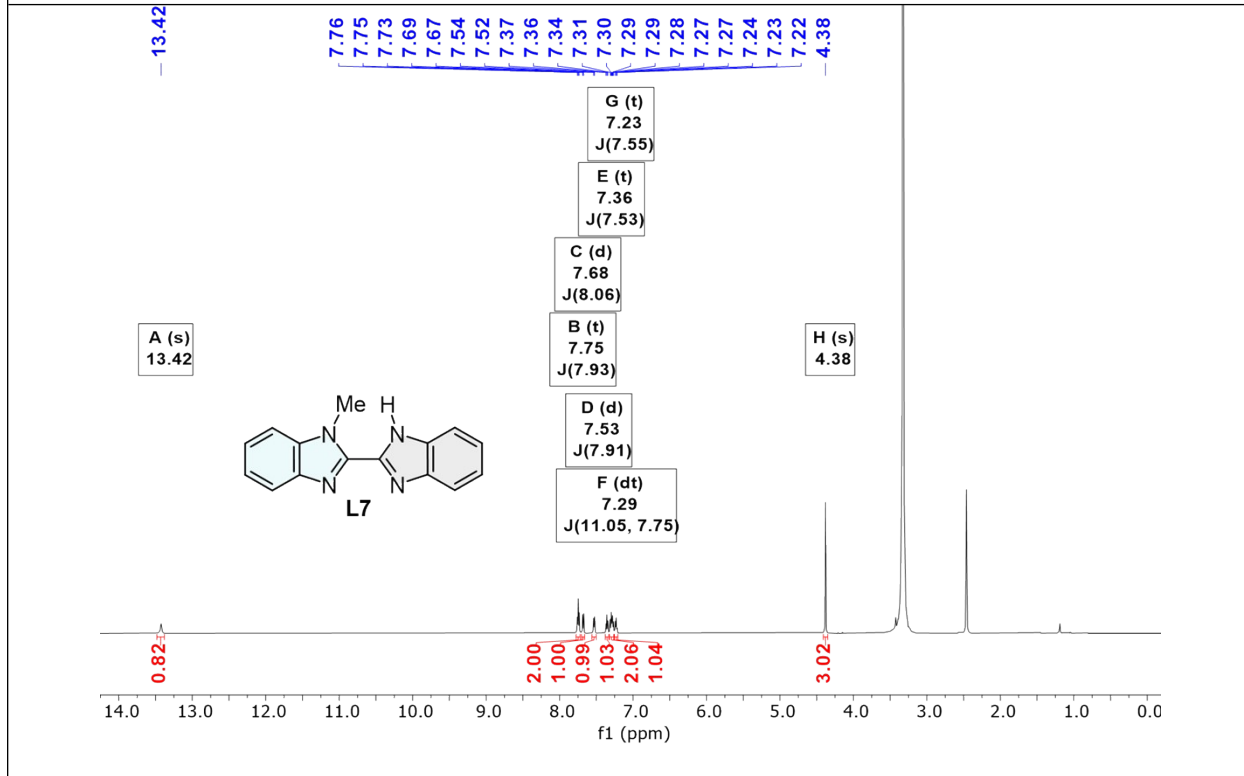
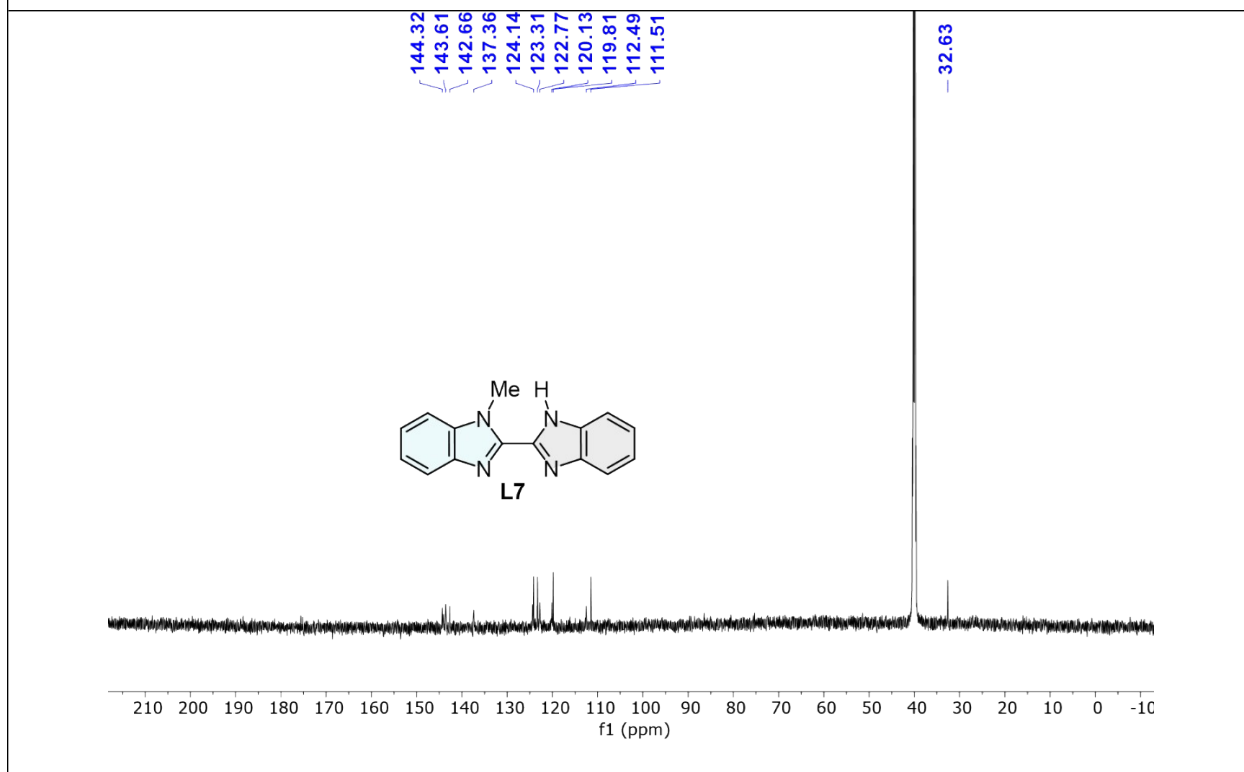
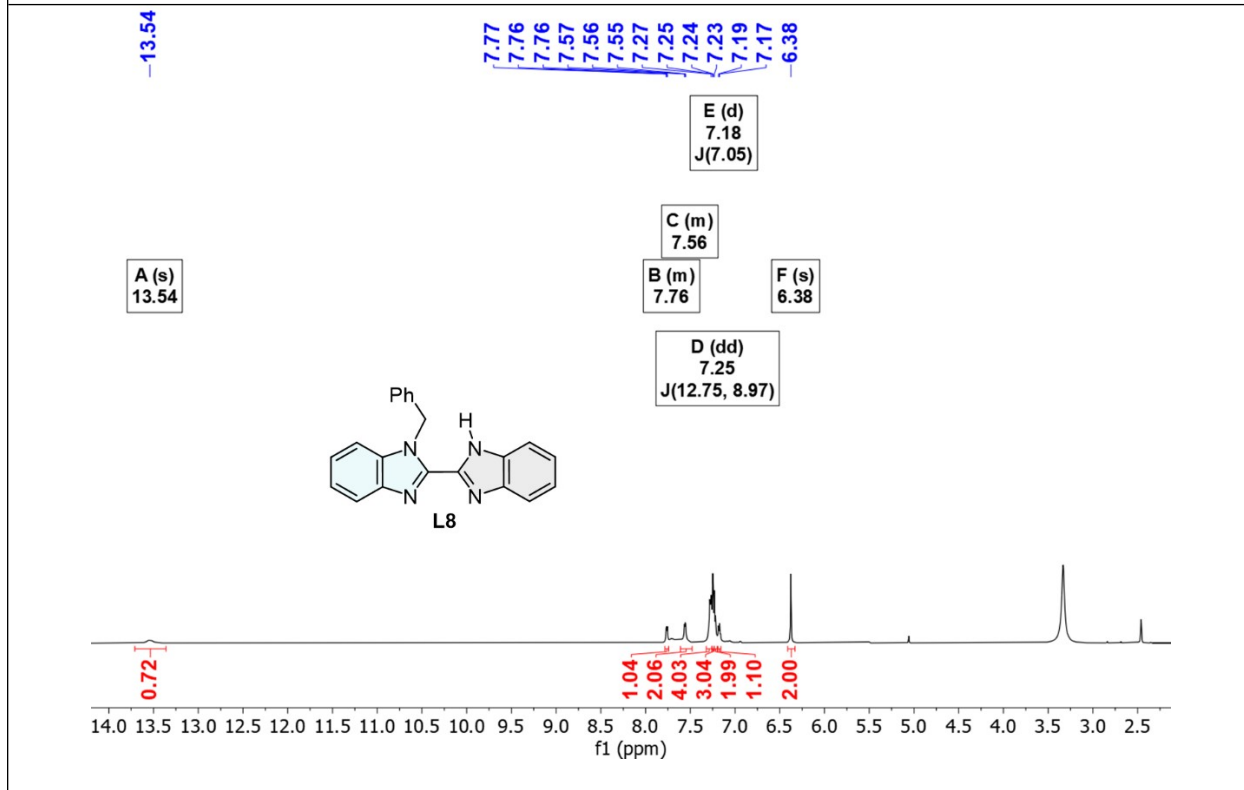


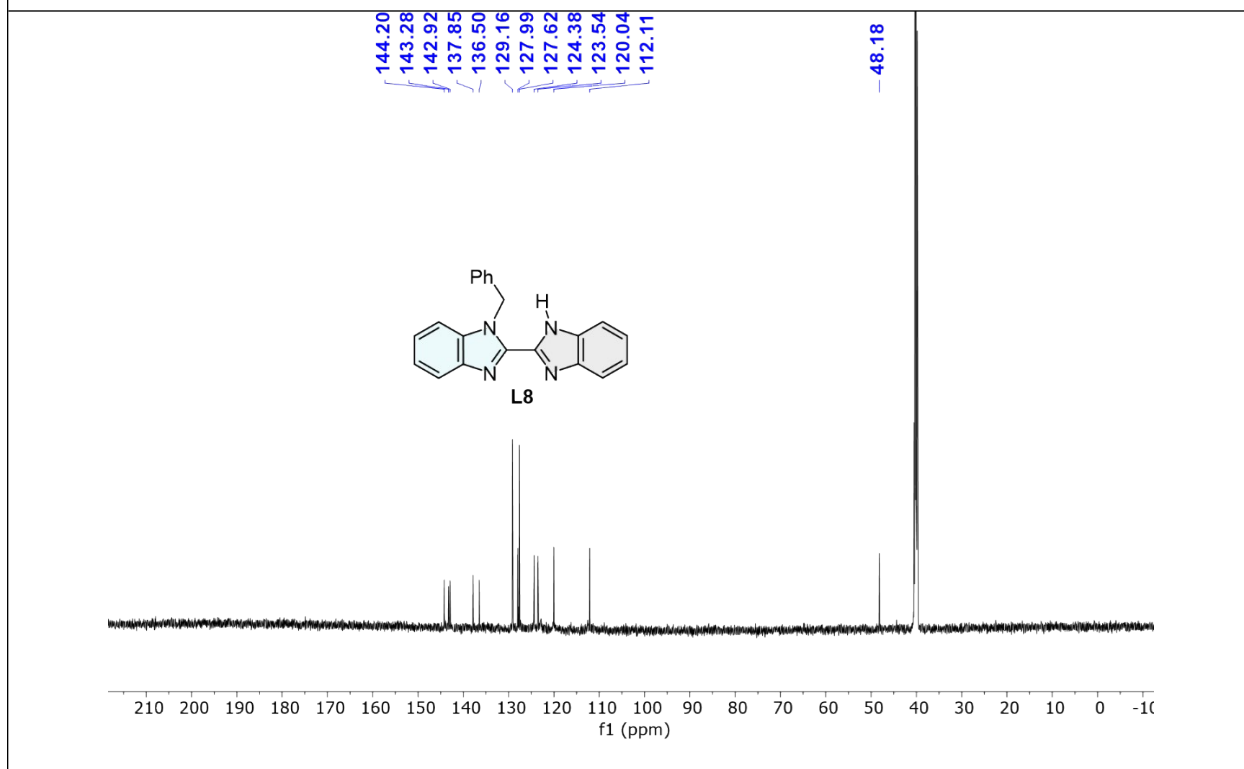
Fig. S29  $^1\text{H}$  NMR spectra of L-7 in DMSO- $d_6$  at 298K.



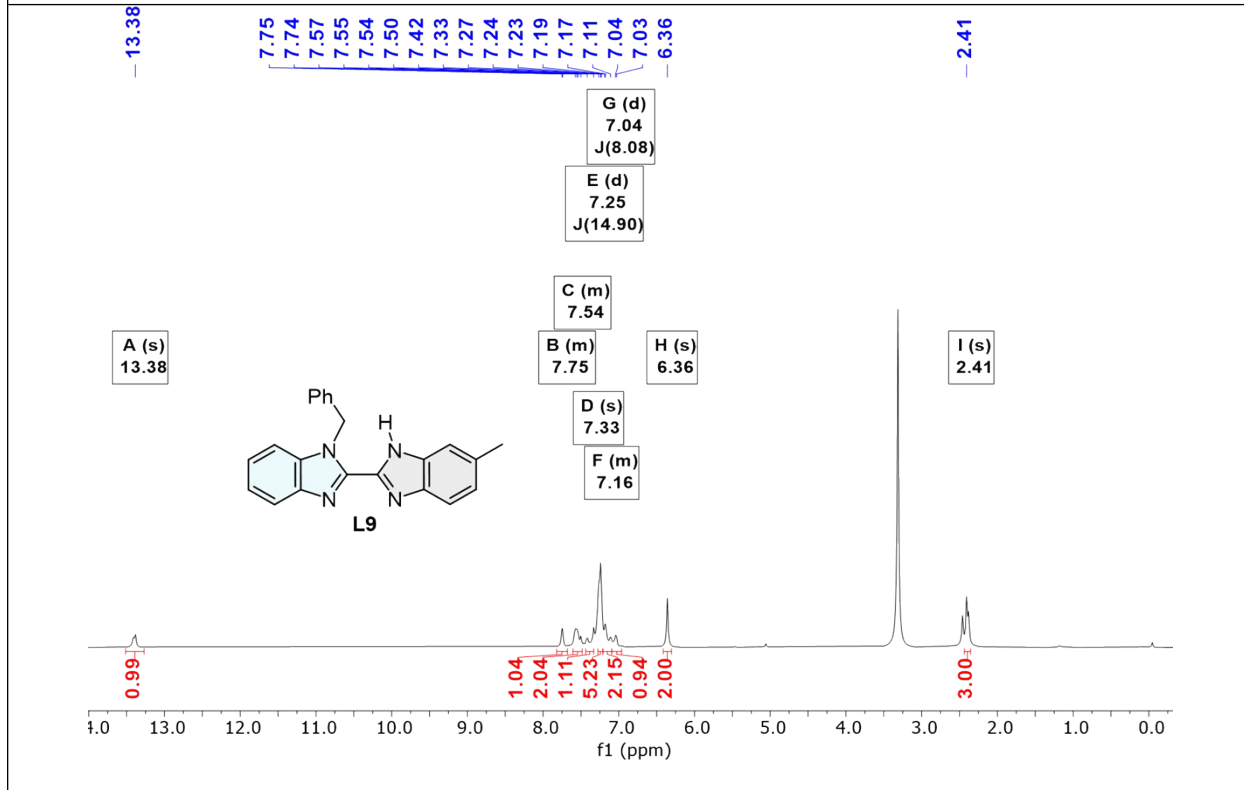
**Fig. S30**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectra of **L-7** in  $\text{DMSO-d}_6$  at 298K.



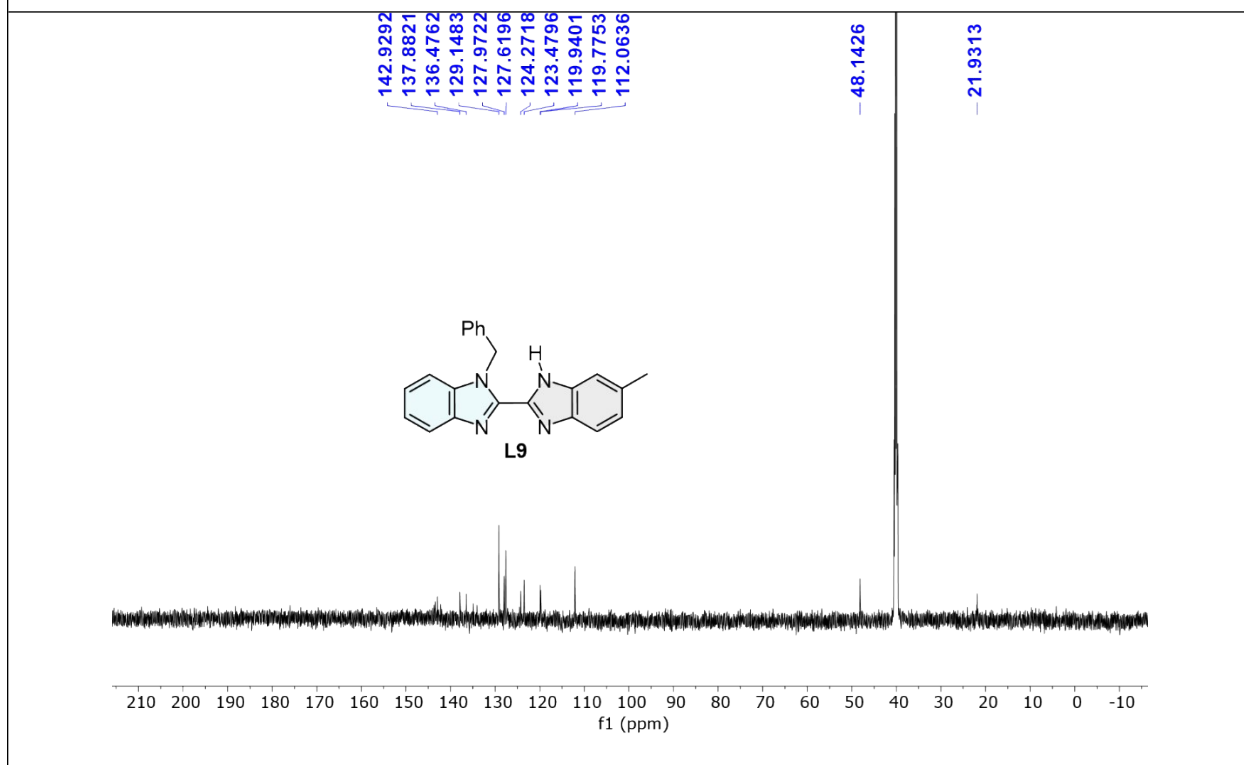
**Fig. S31**  $^1\text{H}$  NMR spectra of **L-8** in  $\text{DMSO-d}_6$  at 298K.



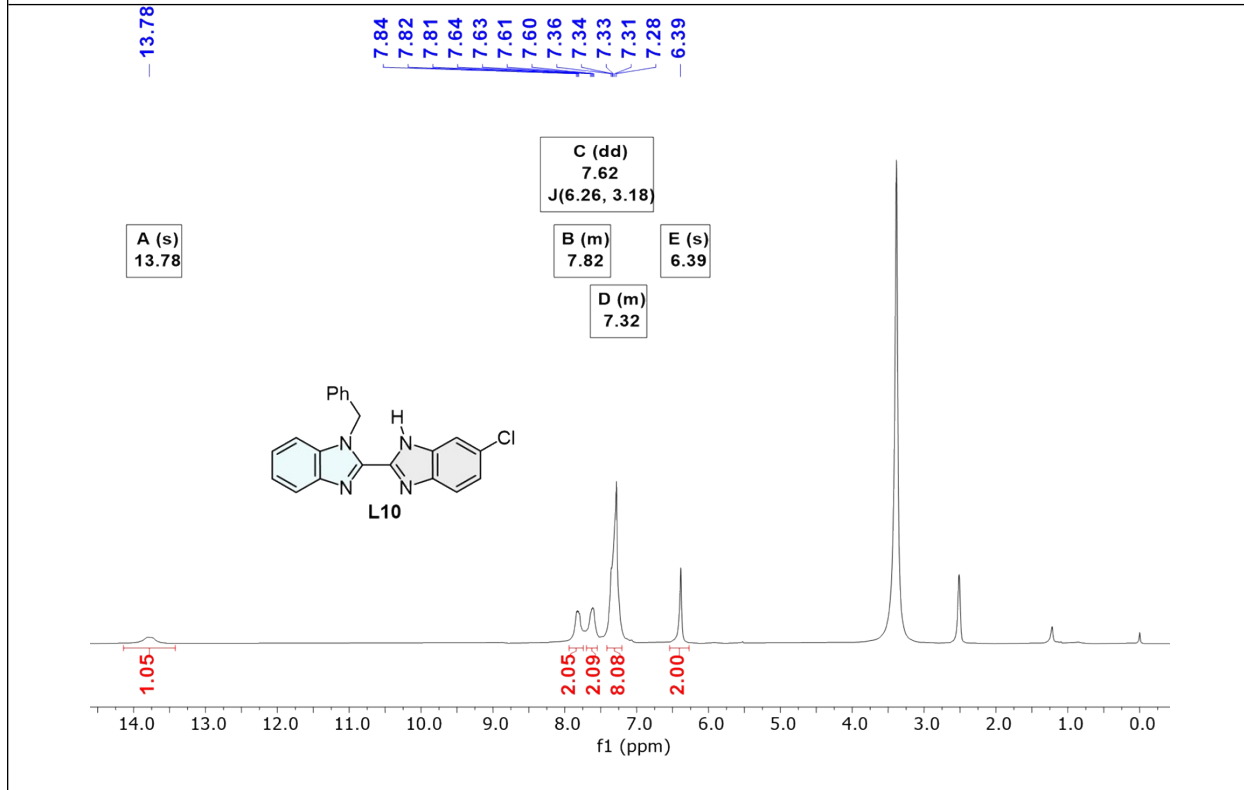
**Fig. S32**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectra of **L-8** in  $\text{DMSO-d}_6$  at 298K.



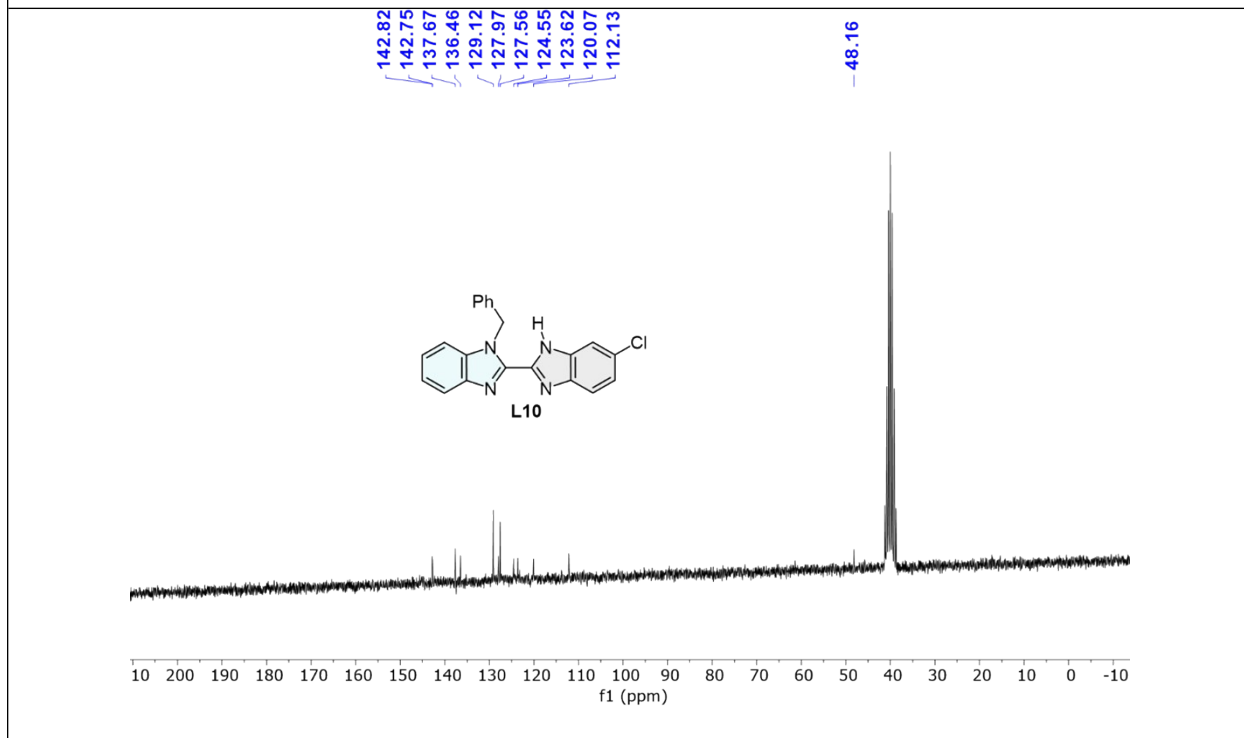
**Fig. S33**  $^1\text{H}$  NMR spectra of **L-9** in  $\text{DMSO-d}_6$  at 298K.



**Fig. S34**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectra of **L-9** in  $\text{DMSO-d}_6$  at 298K.

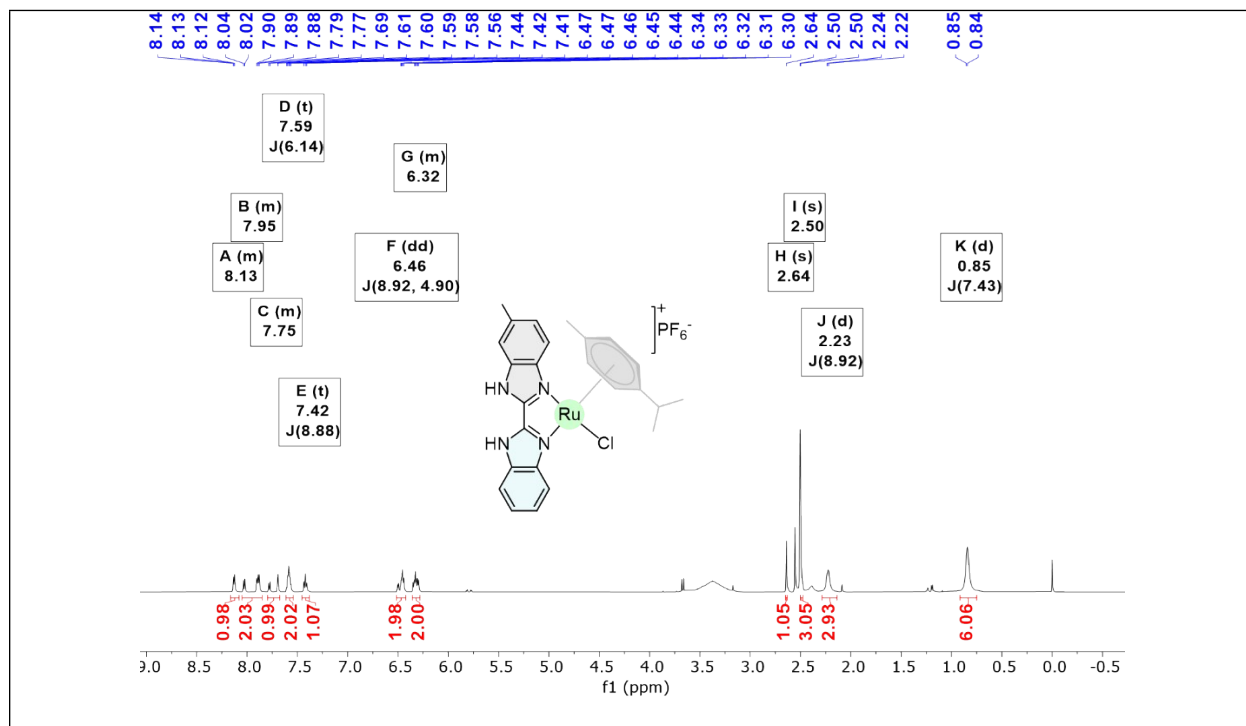


**Fig. S35**  $^1\text{H}$  NMR spectra of **L-10** in  $\text{DMSO-d}_6$  at 298K.



**Fig. S36**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectra of **L-10** in  $\text{DMSO-d}_6$  at 298K.

## 2.2 $^1\text{H}$ and $^{13}\text{C}$ spectra of complexes (Ru5 to Ru10)



**Fig. S37**  $^1\text{H}$  NMR spectra of **Ru-5** in  $\text{DMSO-d}_6$  at 298K.

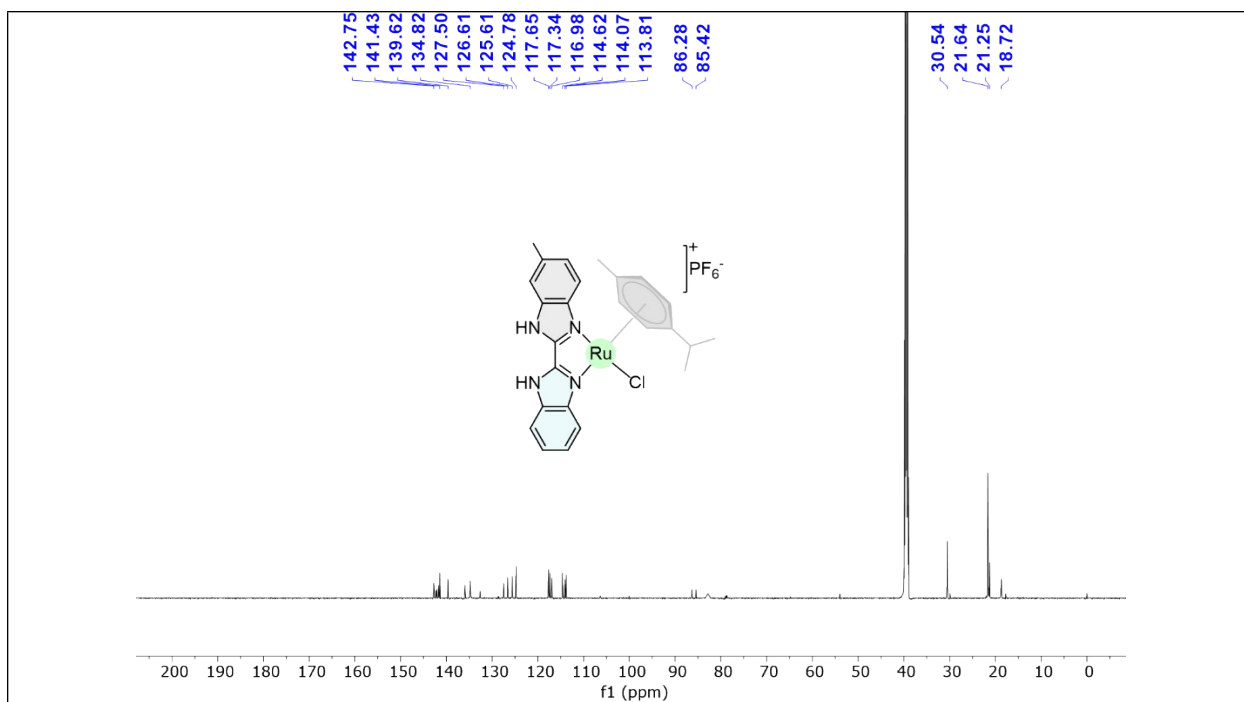


Fig. S38  $^{13}\text{C}\{^1\text{H}\}$  NMR spectra of **Ru-5** in DMSO- $d_6$  at 298K.

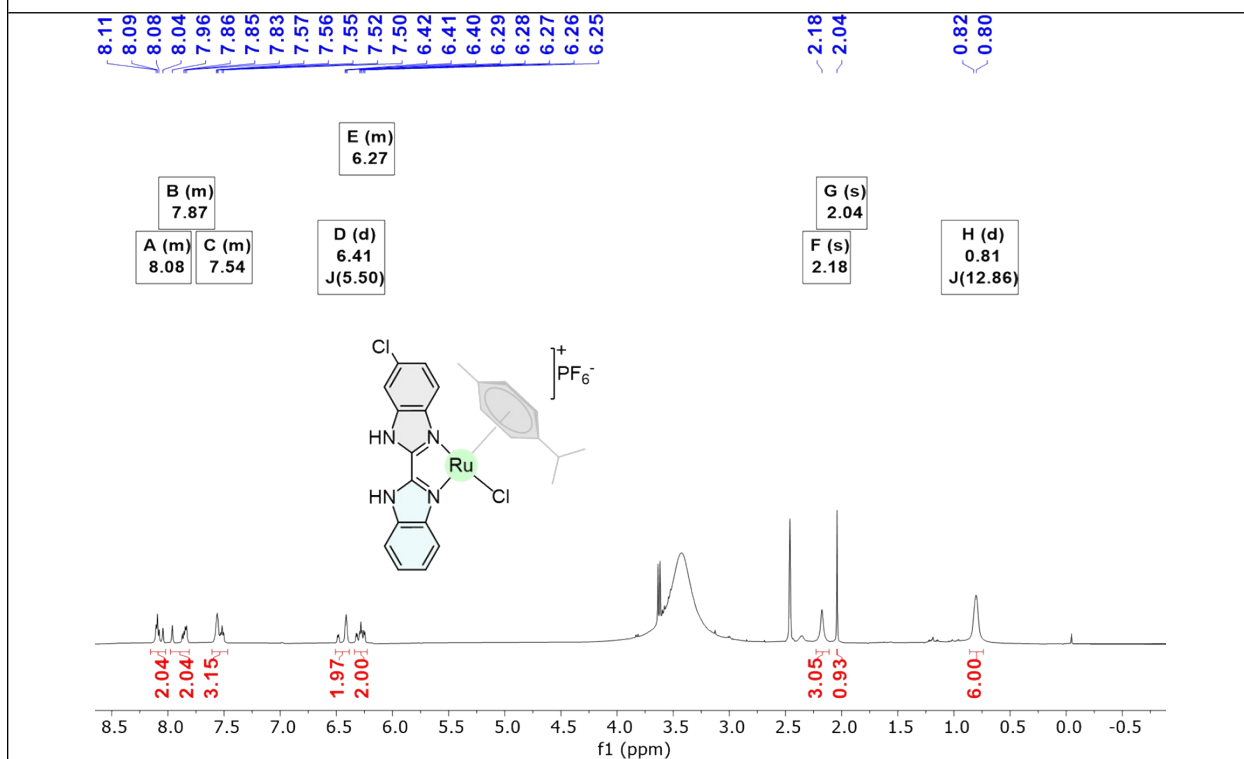


Fig. S39  $^1\text{H}$  NMR spectra of **Ru-6** in DMSO- $d_6$  at 298K.

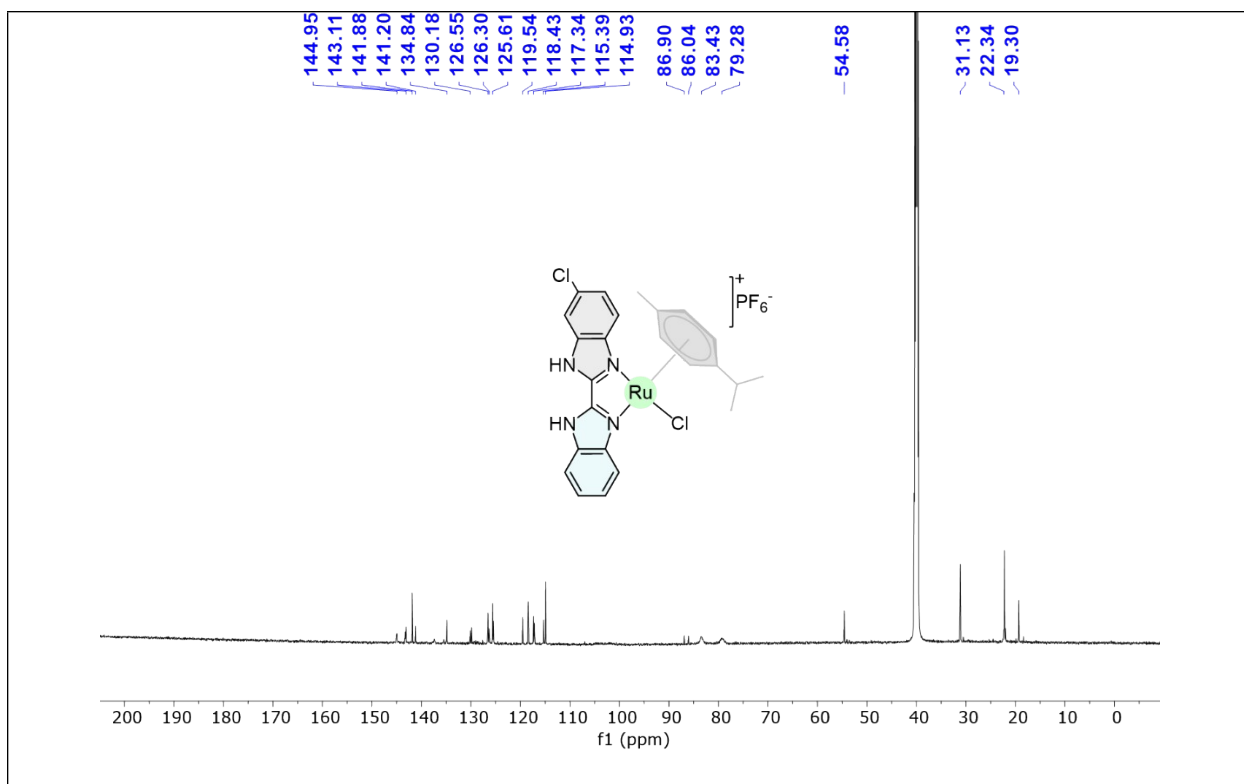


Fig. S40 <sup>13</sup>C {<sup>1</sup>H} NMR spectra of Ru-6 in DMSO-d<sub>6</sub> at 298K.

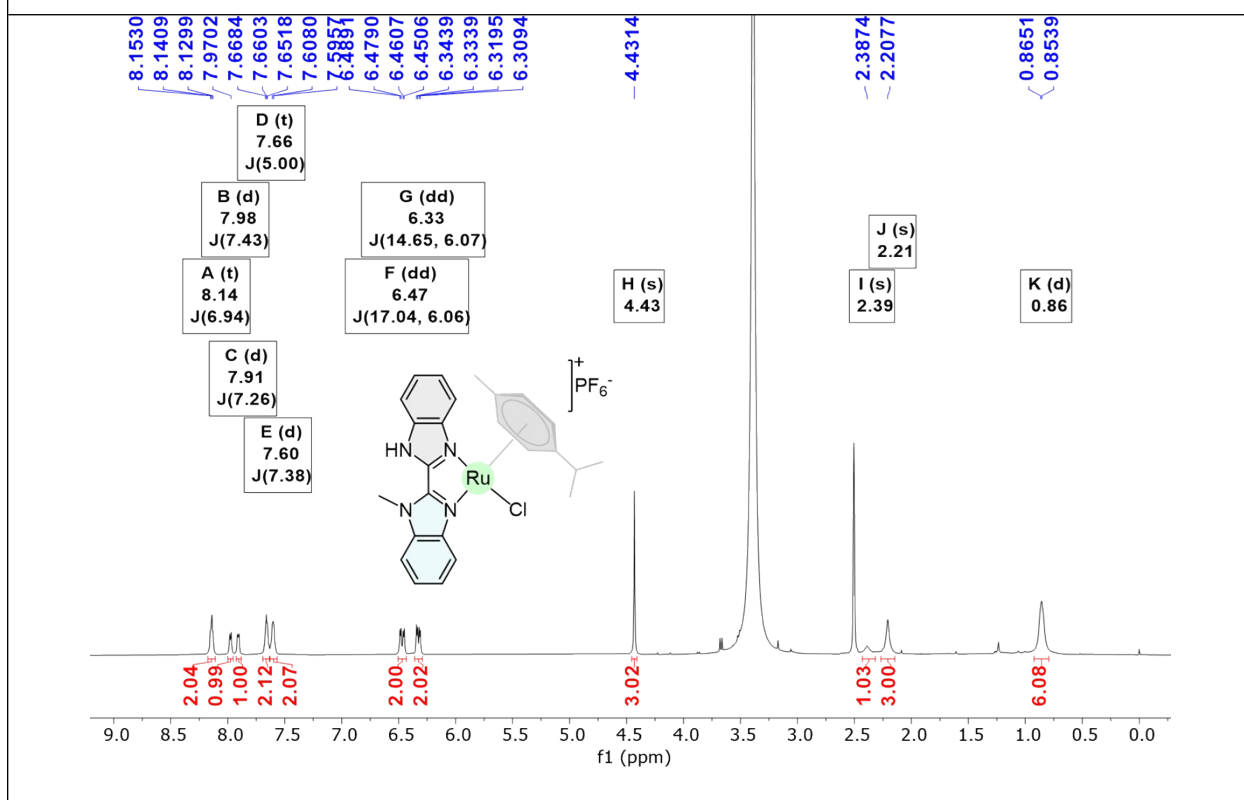


Fig. S41 <sup>1</sup>H NMR spectra of Ru-7 in DMSO-d<sub>6</sub> at 298K.

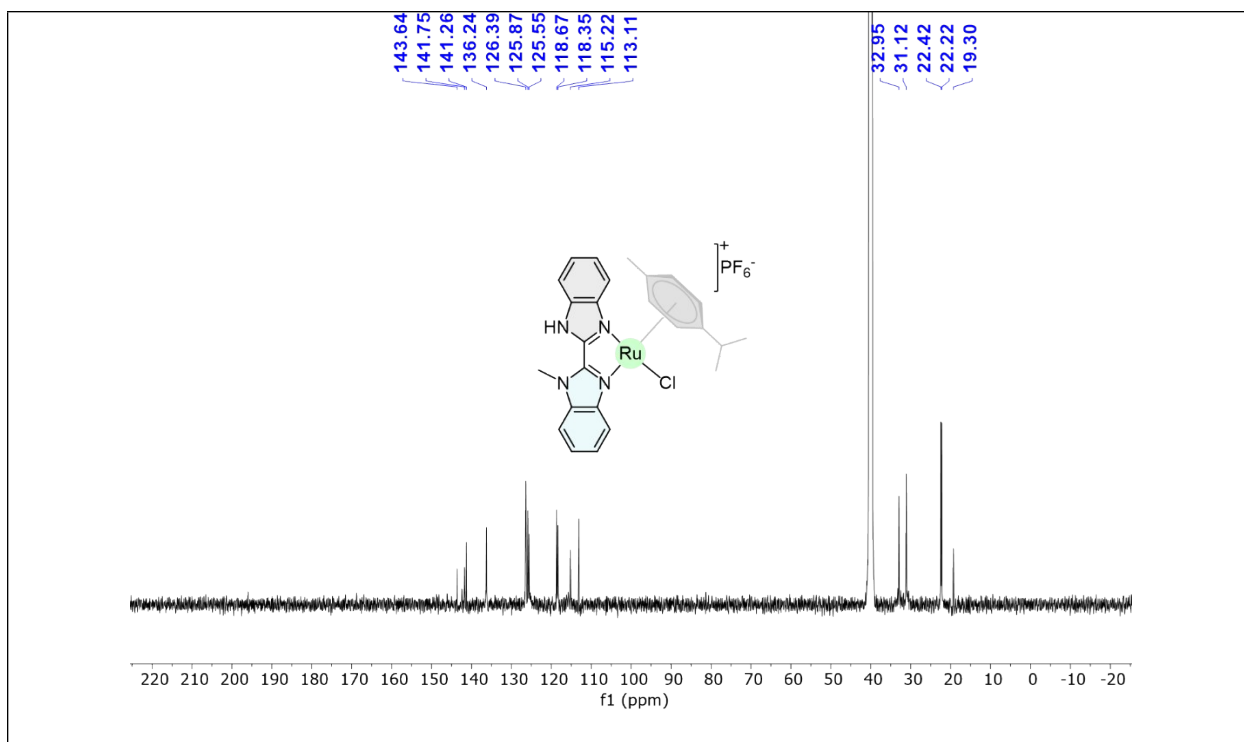


Fig. S42  $^{13}\text{C}\{^1\text{H}\}$  NMR spectra of **Ru-7** in DMSO- $d_6$  at 298K.

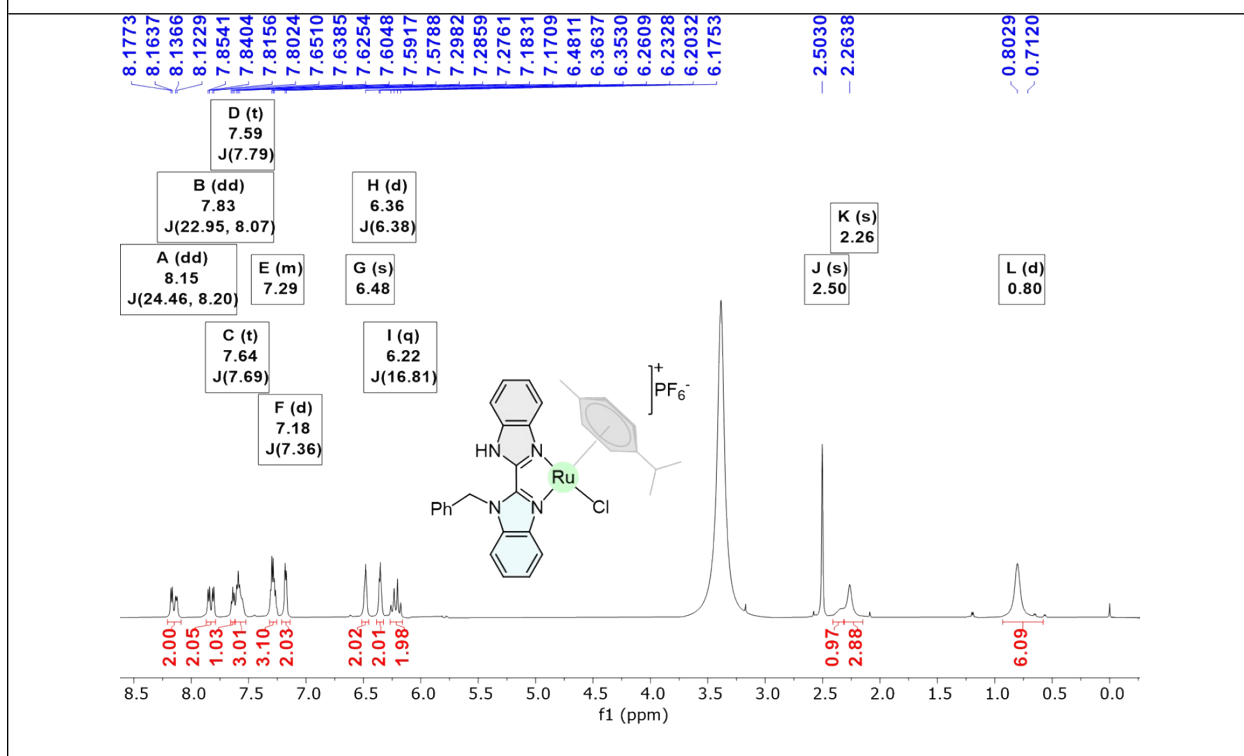


Fig. S43  $^1\text{H}$  NMR spectra of **Ru-8** in DMSO- $d_6$  at 298K.

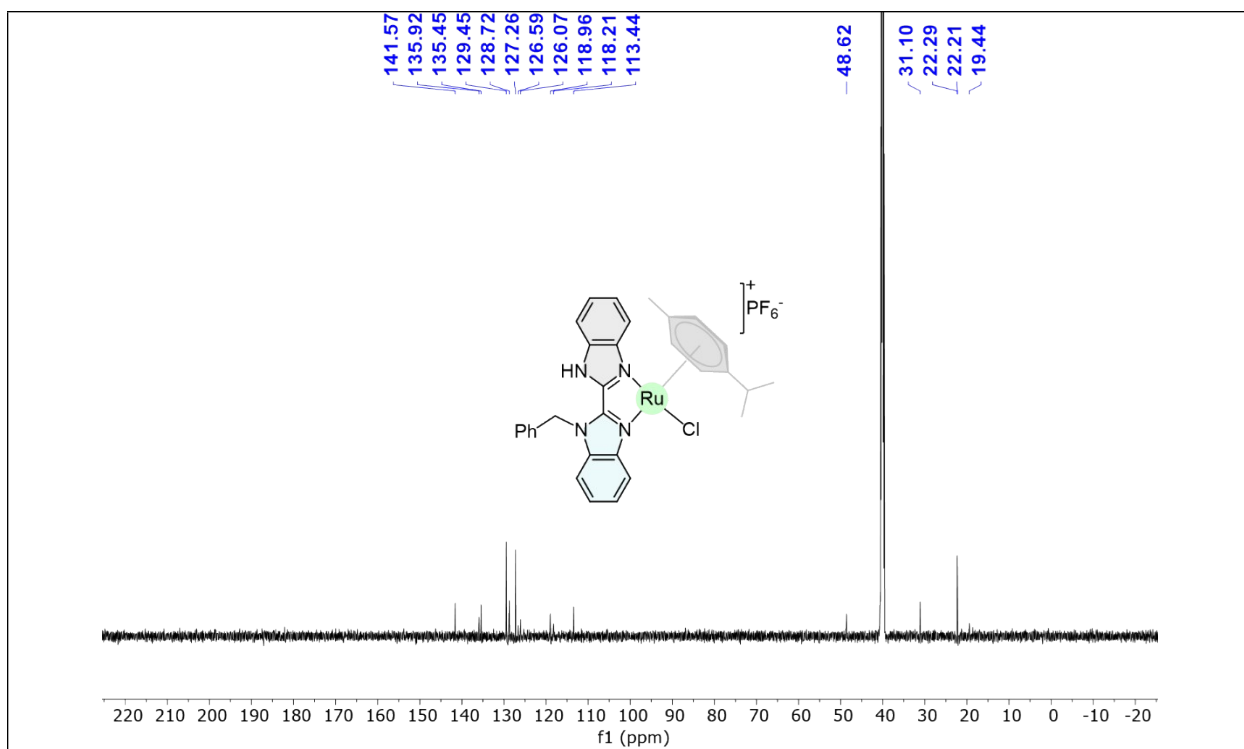


Fig. S44 <sup>13</sup>C {<sup>1</sup>H} NMR spectra of **Ru-8** in DMSO-d<sub>6</sub> at 298K.

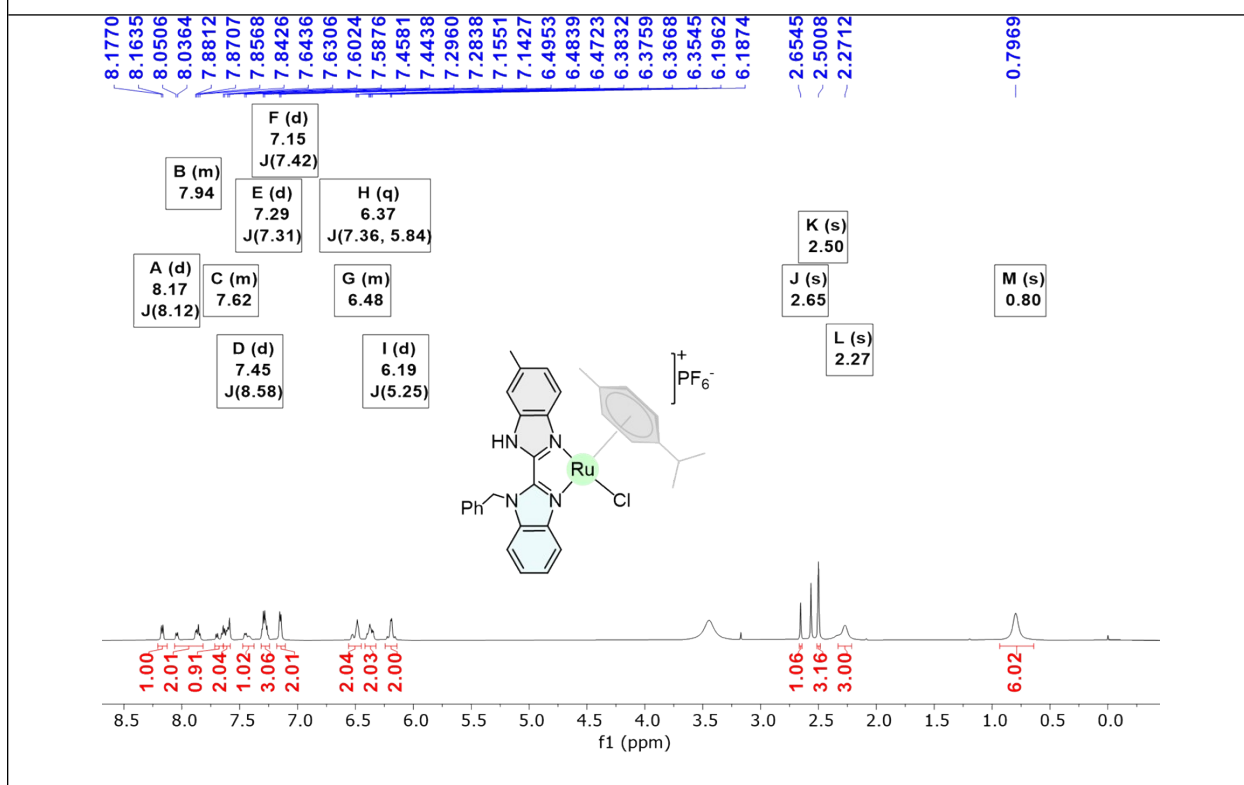


Fig. S45 <sup>1</sup>H NMR spectra of **Ru-9** in DMSO-d<sub>6</sub> at 298K.

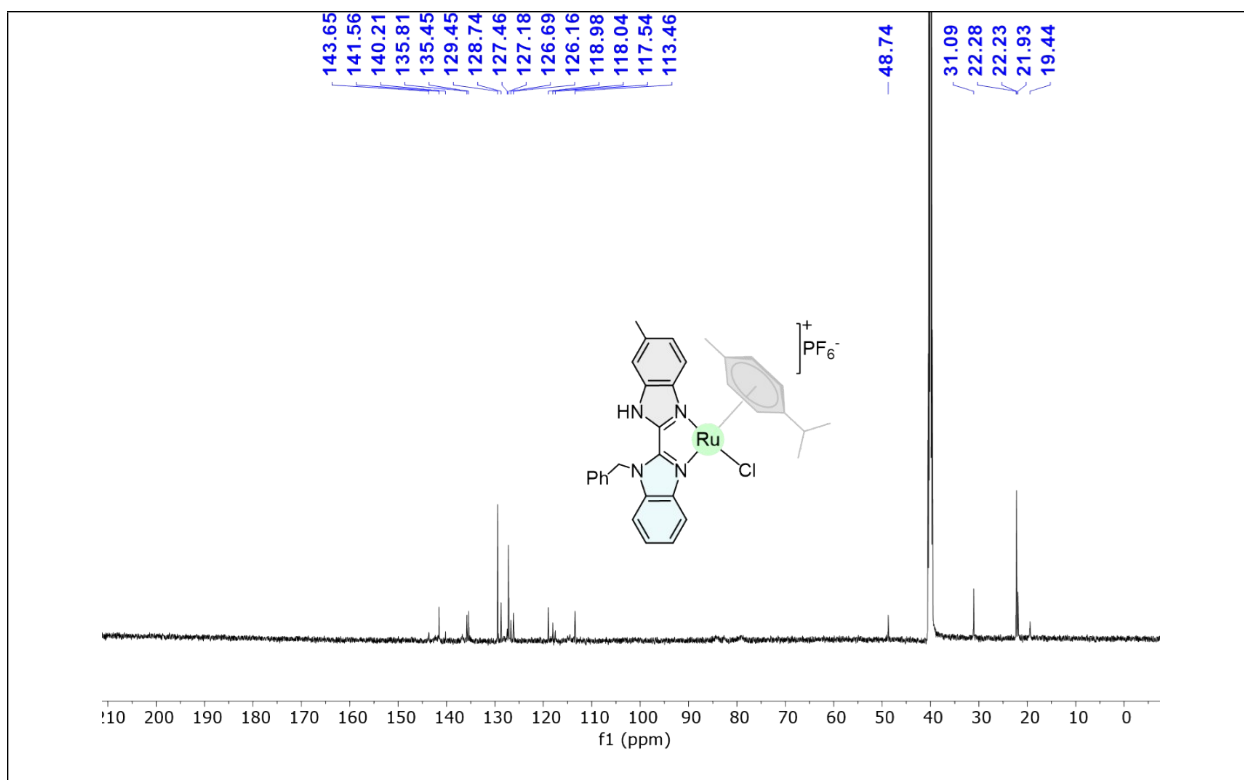


Fig. S46  $^{13}\text{C}\{^1\text{H}\}$  NMR spectra of **Ru-9** in DMSO- $\text{d}_6$  at 298K.

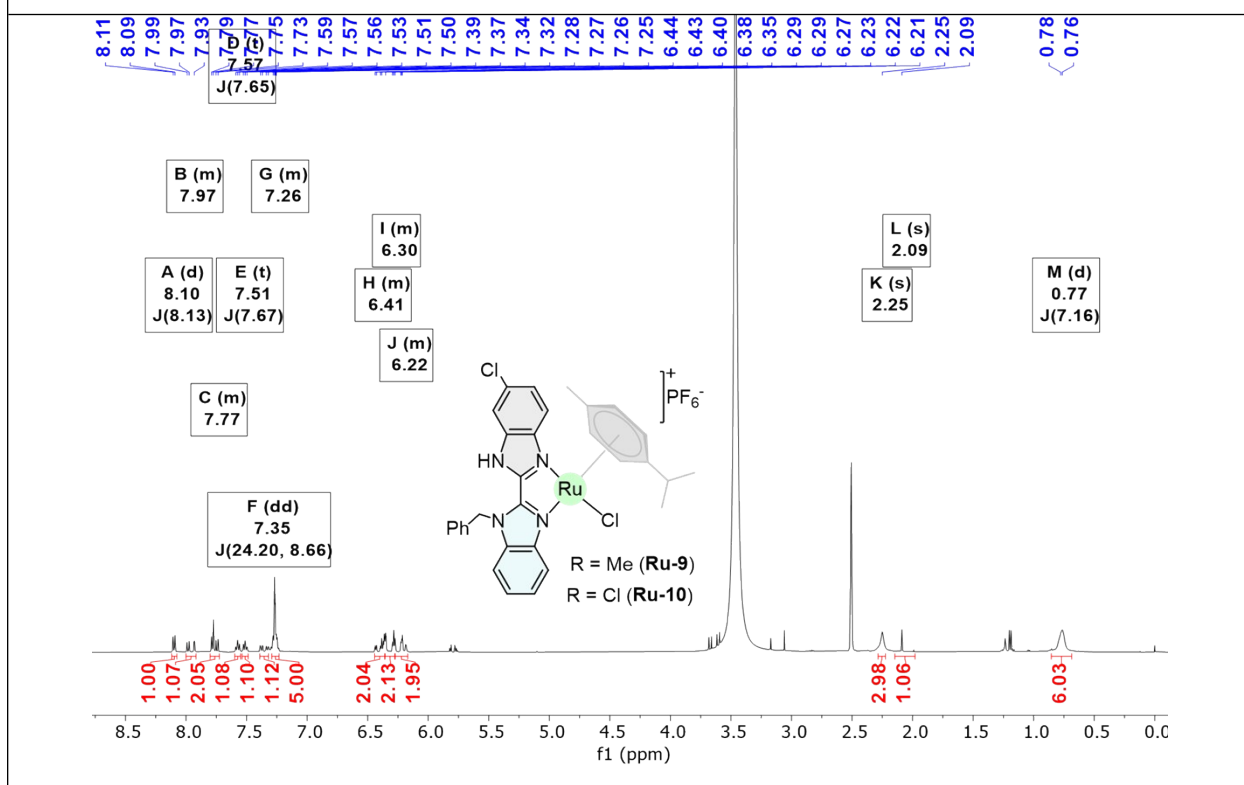
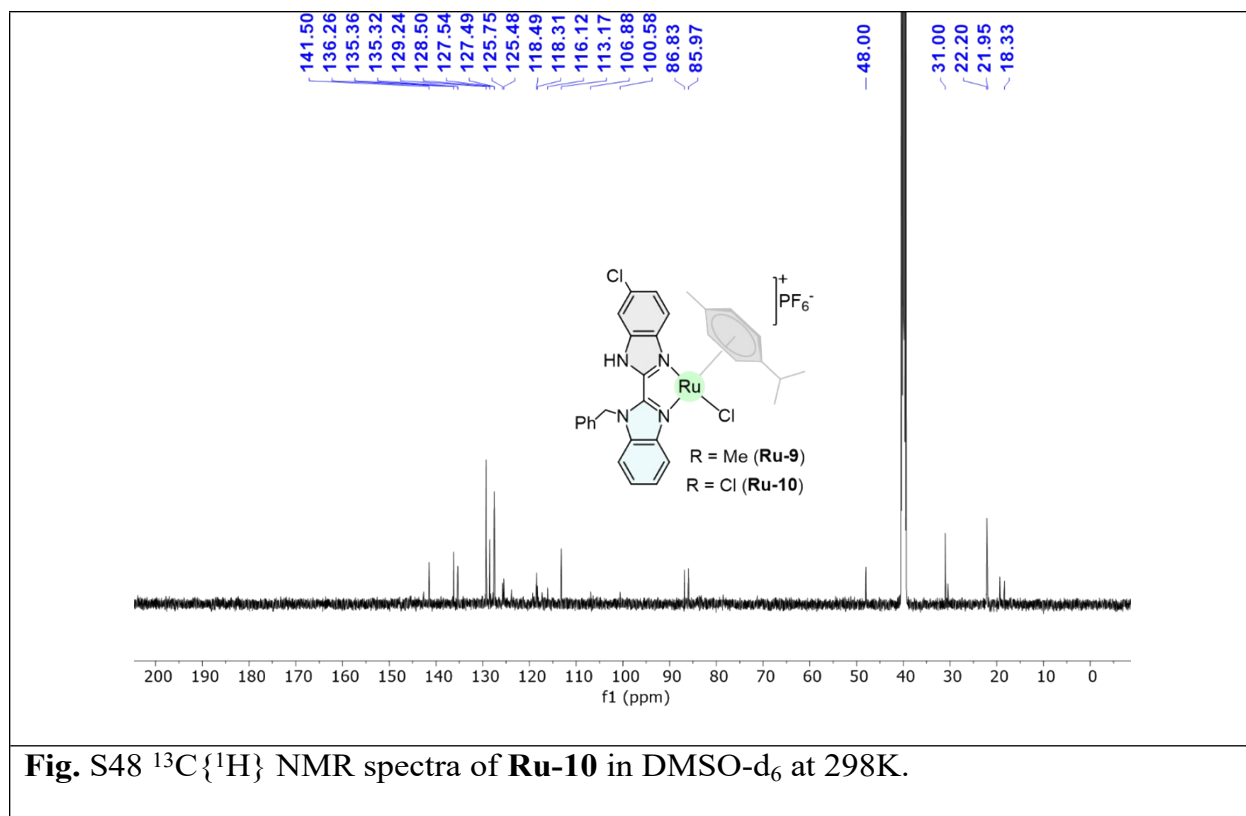


Fig. S47  $^1\text{H}$  NMR spectra of **Ru-10** in DMSO- $\text{d}_6$  at 298K.

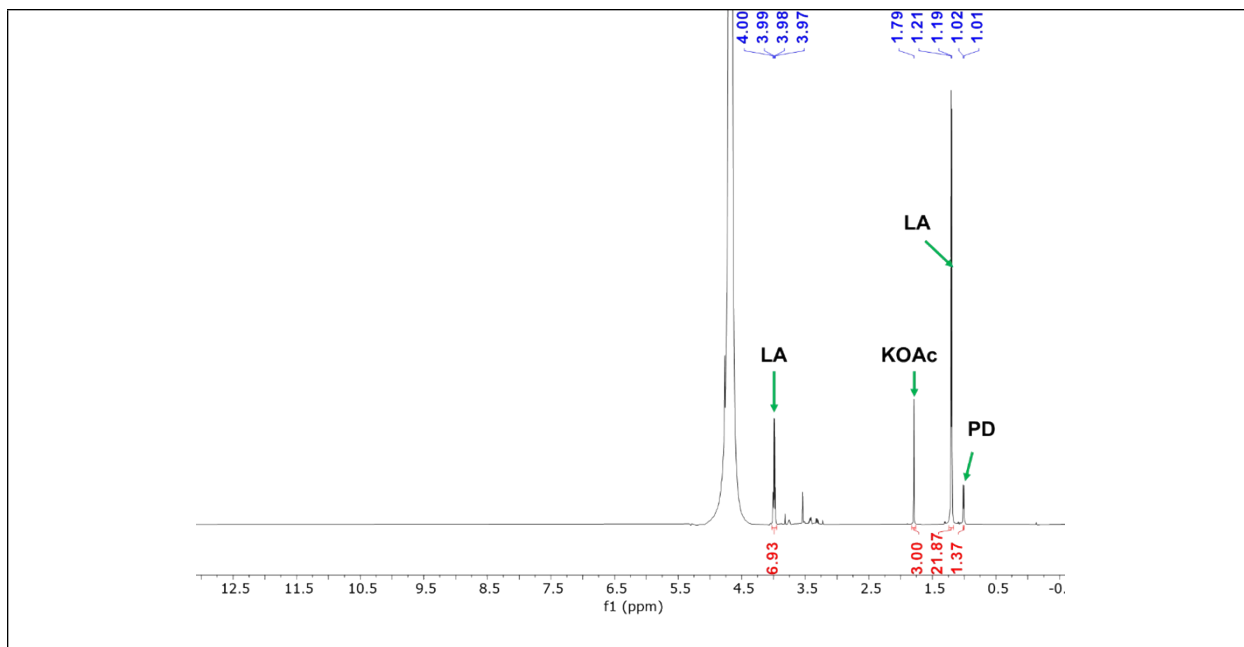


### 3. General procedure and $^1\text{H}$ NMR Spectra of optimizations.

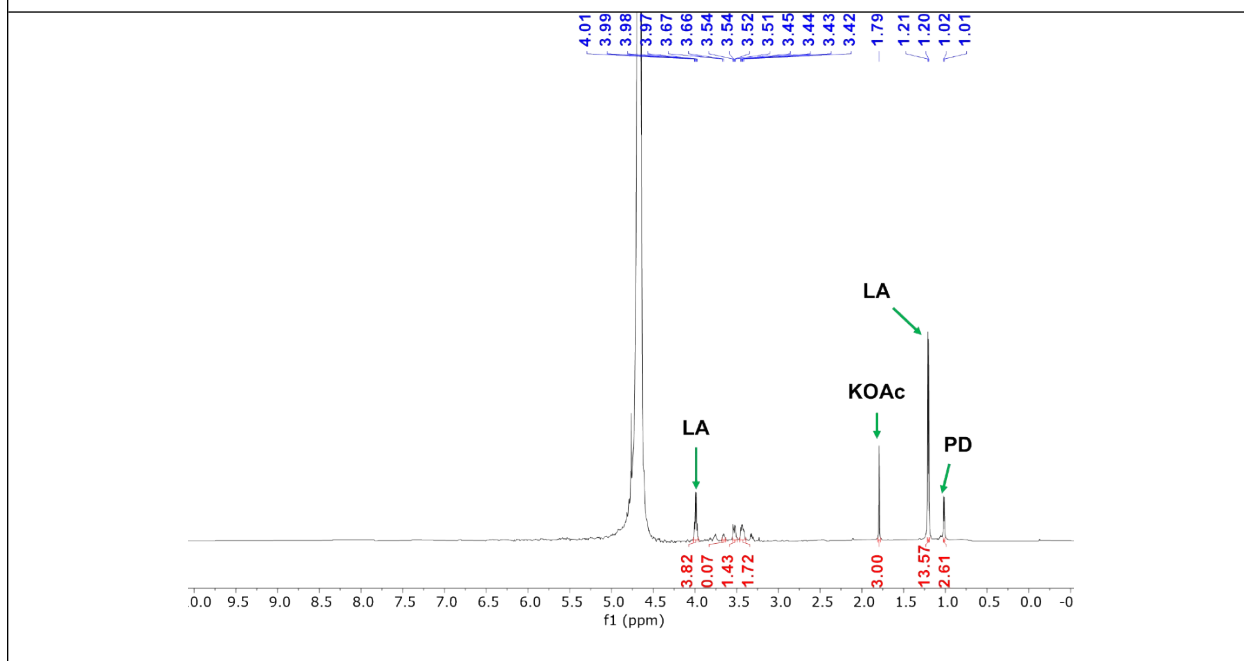
#### General procedure for the catalytic dehydrogenation of glycerol to lactic acid

**Optimized reaction condition:** For this, glycerol (7 mmol; 0.510 mL), water (0.5 mL), NaOH (7 mmol; 0.280 g), and **Ru-1** (0.05 mol%, 2.5 mg) were placed in a 20 mL glass tube and heated at 160 °C for 24 h. After completion, 5 mL of water was added to the reaction mixture. The conversion of glycerol and the selectivity toward lactic acid (**LA**) were determined by  $^1\text{H}$  NMR spectroscopy in  $\text{D}_2\text{O}$  solvent, using KOAc as an external standard.

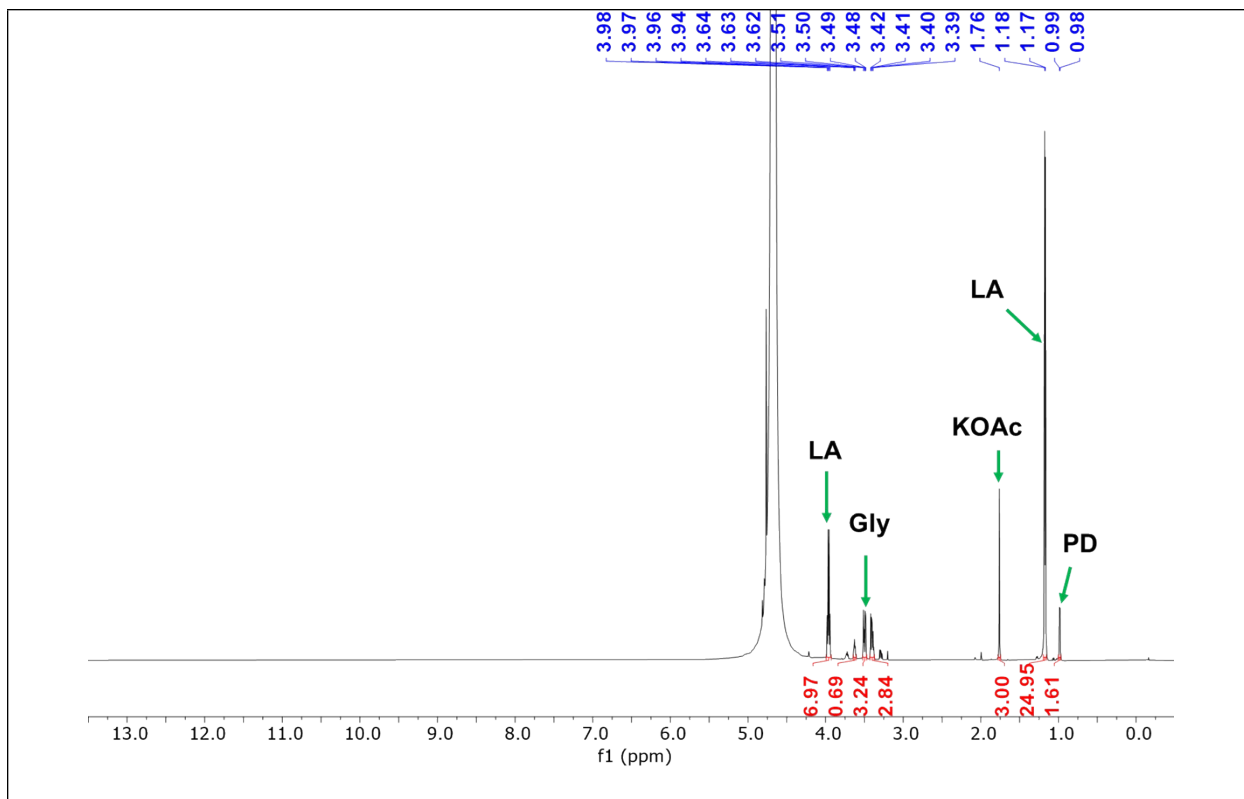
#### 3.1 Base Optimization



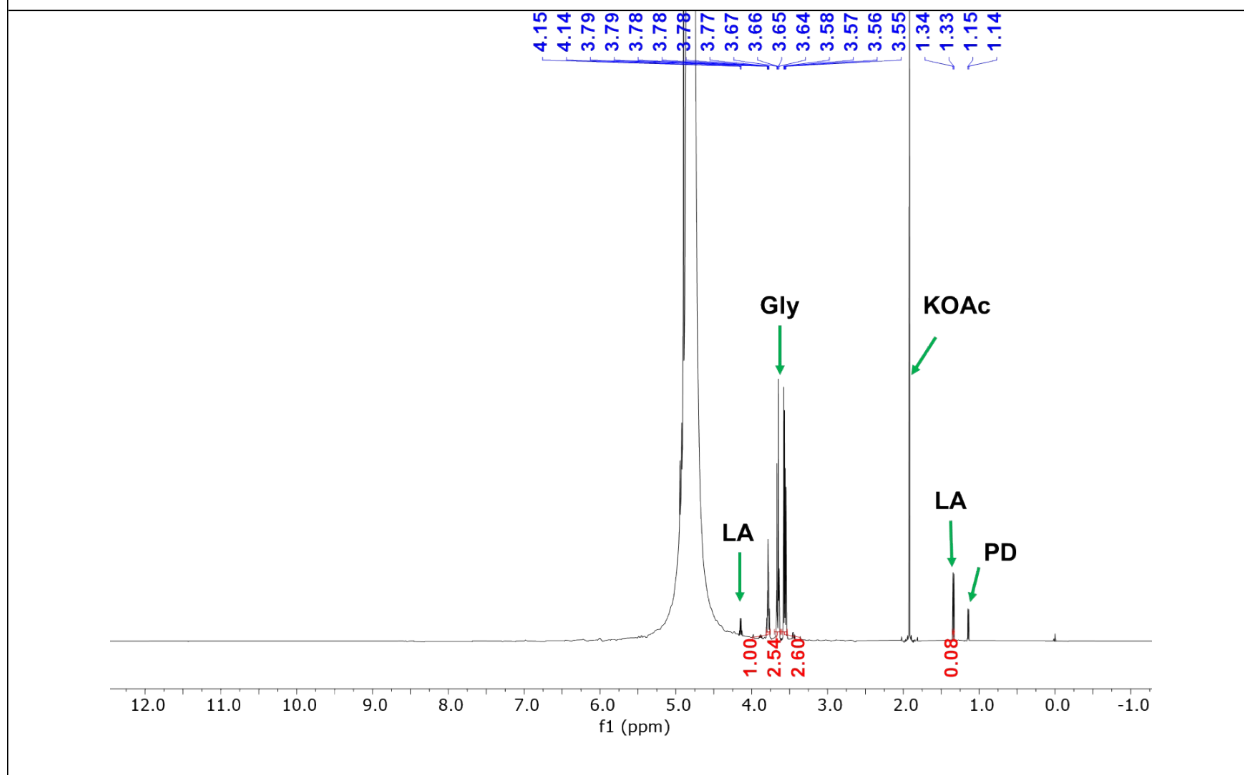
**Fig. S49**  $^1\text{H}$  NMR spectra of Gly to LA in NaOH at 298 K in  $\text{D}_2\text{O}$ .



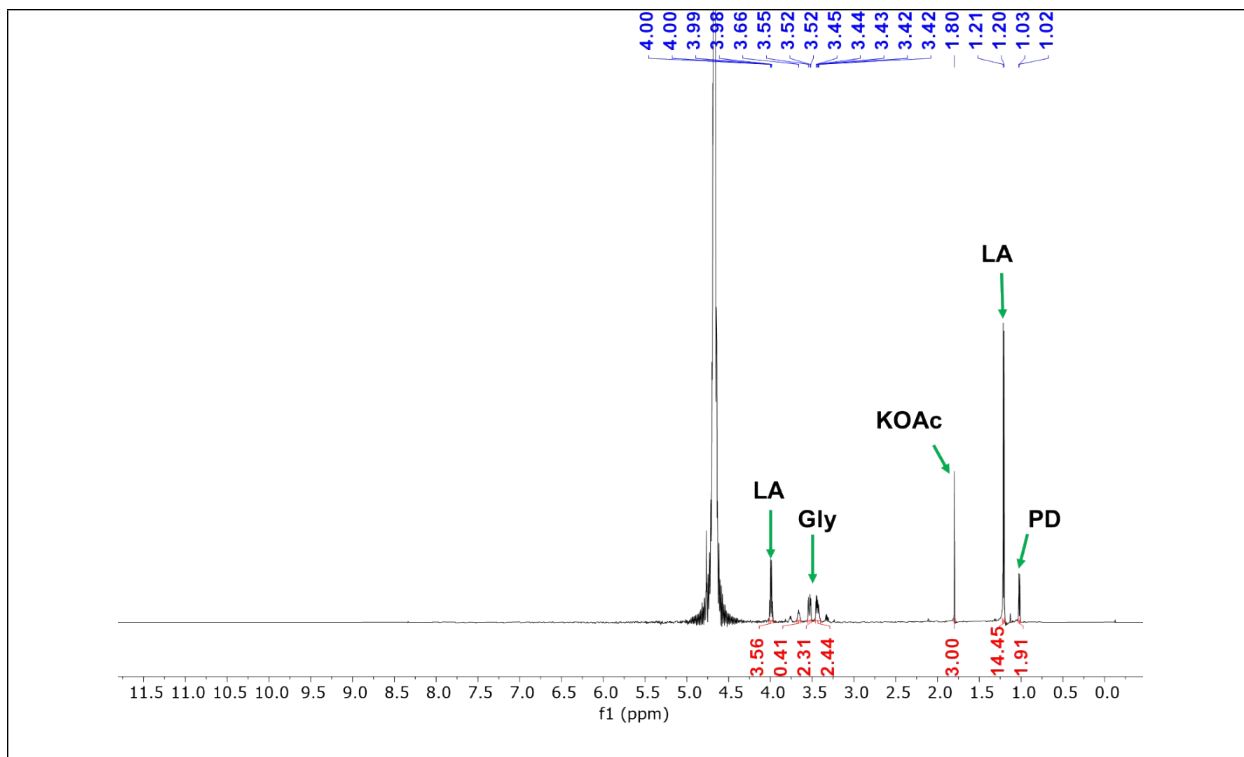
**Fig. S50**  $^1\text{H}$  NMR spectra of Gly to LA in KOH at 298 K in  $\text{D}_2\text{O}$ .



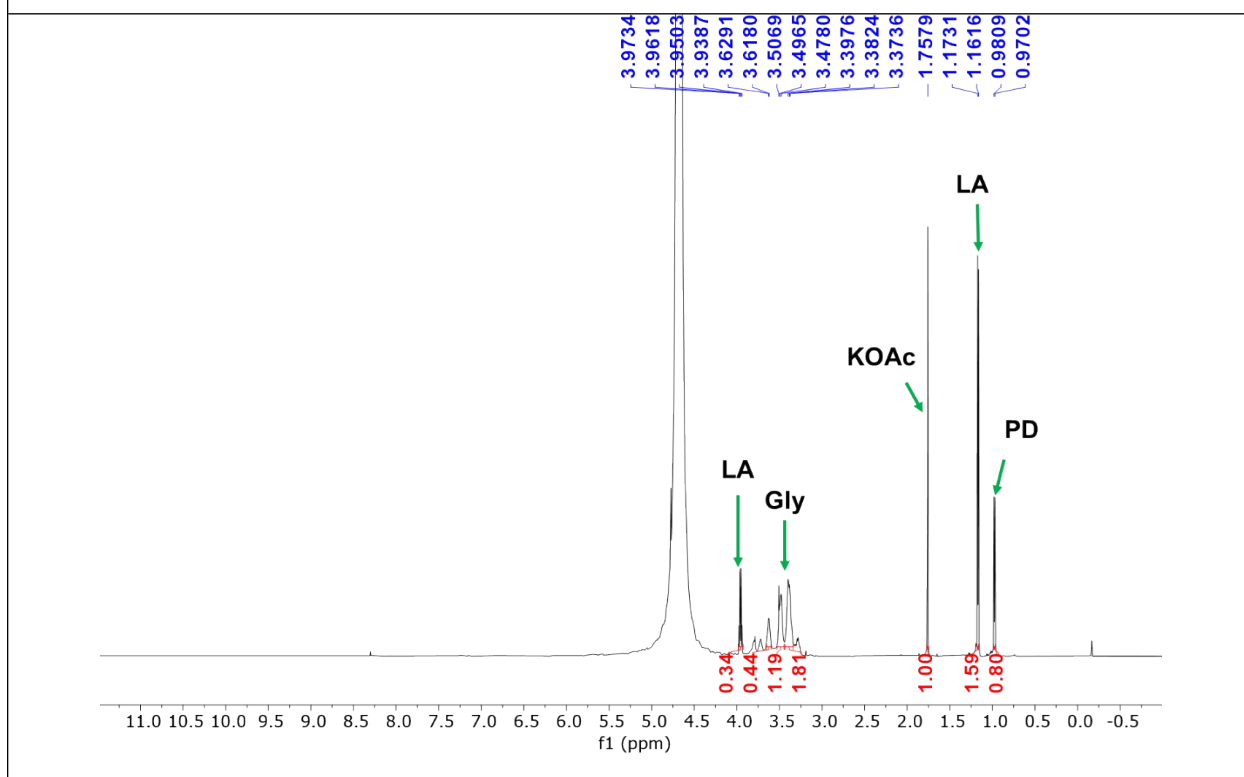
**Fig. S51**  $^1\text{H}$  NMR spectra of **Gly** to **LA** in  $\text{LiOH}$  at 298 K in  $\text{D}_2\text{O}$ .



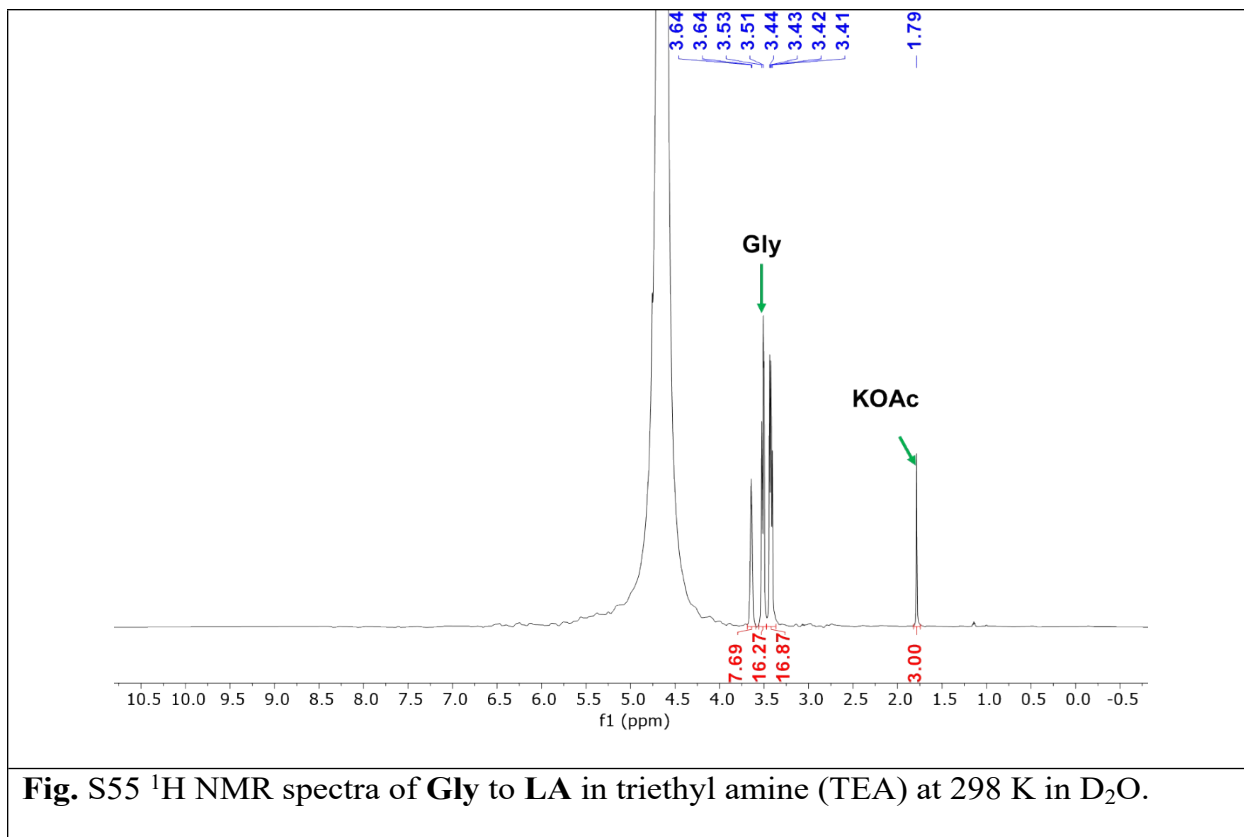
**Fig. S52**  $^1\text{H}$  NMR spectra of **Gly** to **LA** in  $\text{Ca}(\text{OH})_2$  at 298 K in  $\text{D}_2\text{O}$ .



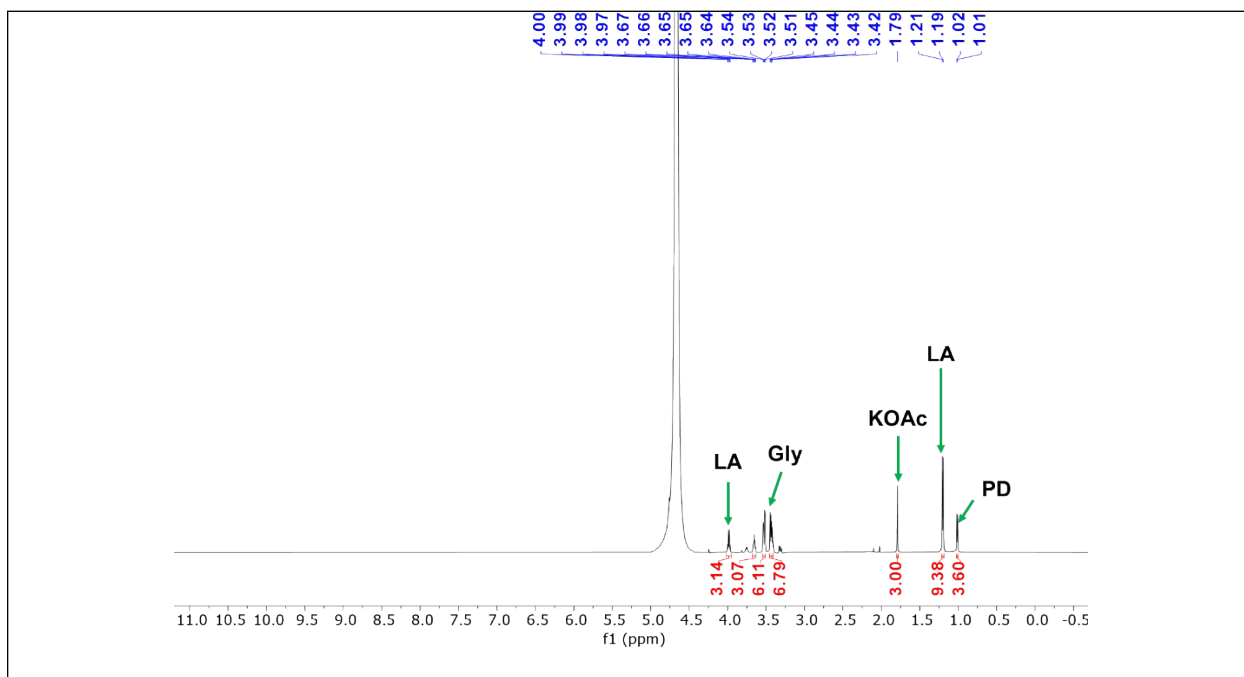
**Fig. S53**  $^1\text{H}$  NMR spectra of **Gly** to **LA** in  $\text{K}'\text{OBu}$  at 298 K in  $\text{D}_2\text{O}$ .



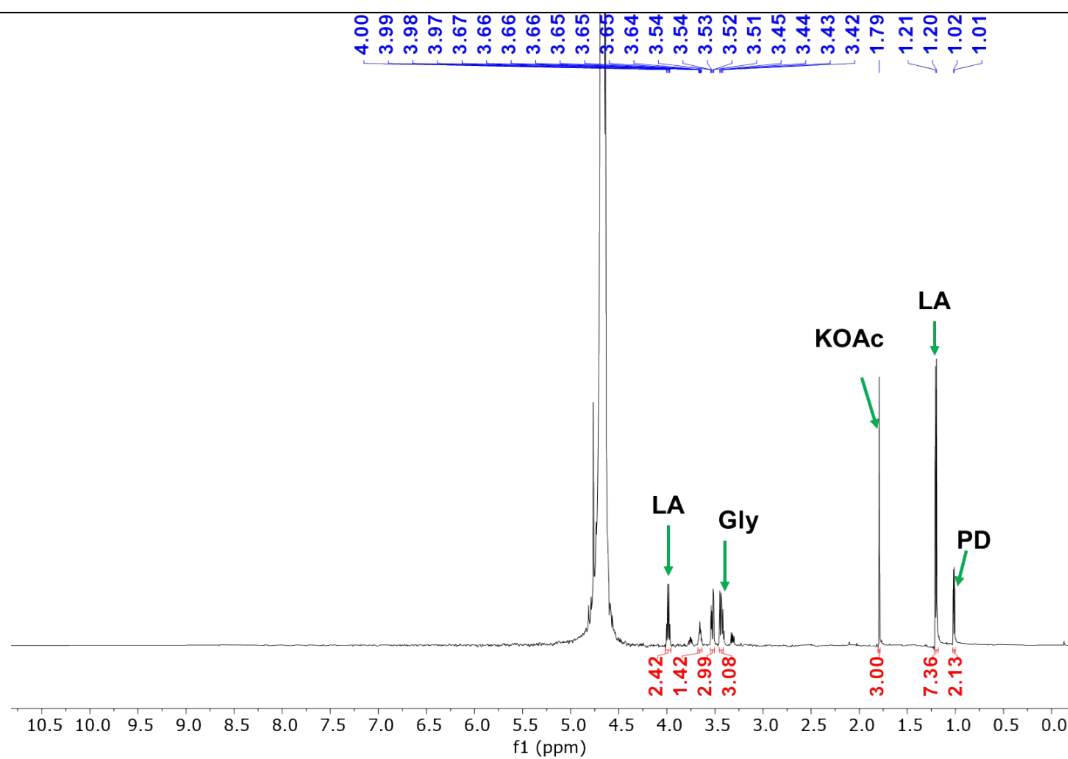
**Fig. S54**  $^1\text{H}$  NMR spectra of **Gly** to **LA** in  $\text{NaOMe}$  at 298 K in  $\text{D}_2\text{O}$ .



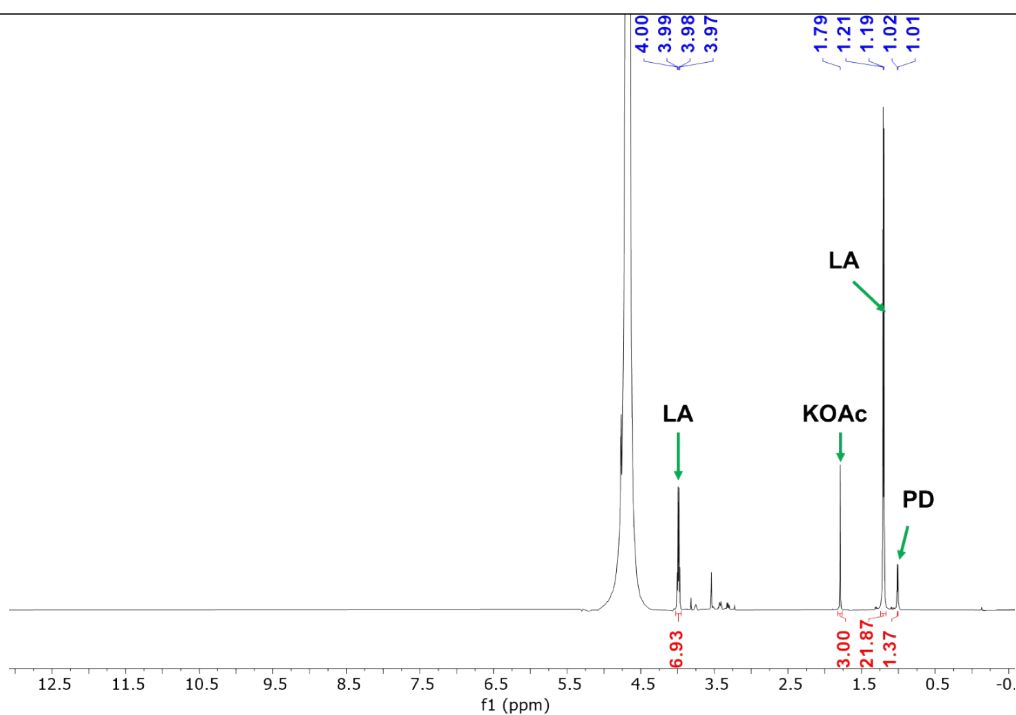
### 3.2 Ru-1 mol% Optimization



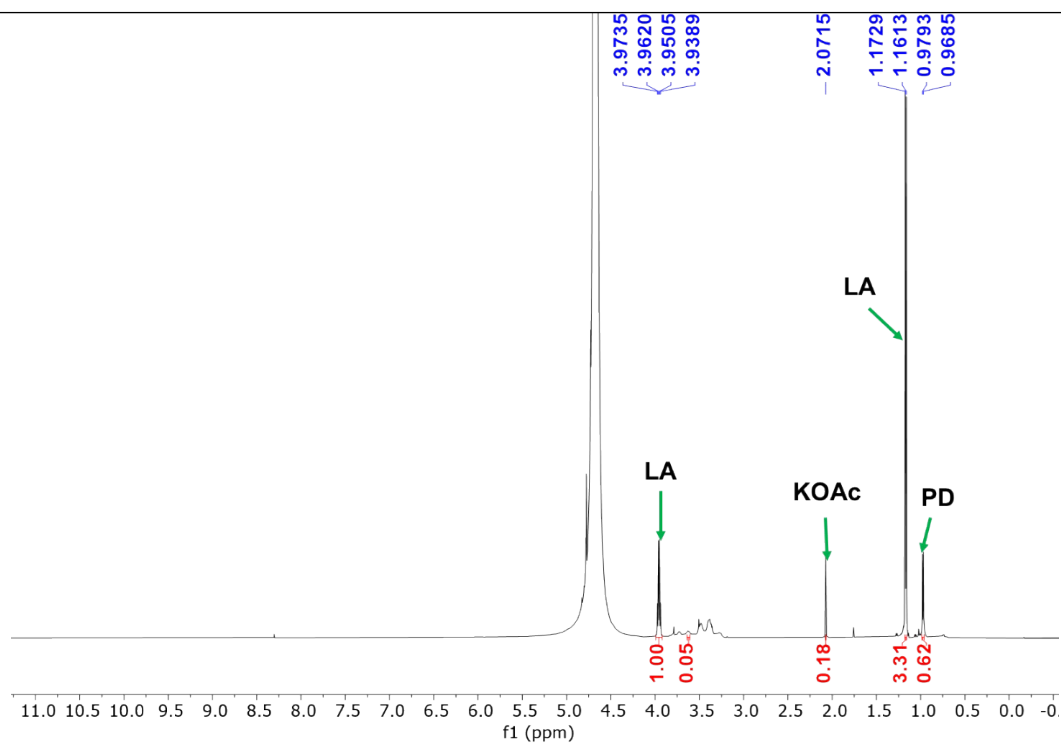
**Fig. S56**  $^1\text{H}$  NMR spectra of **Gly** to **LA** at 0.01 mol% of **Ru-1** at 298 K in  $\text{D}_2\text{O}$ .



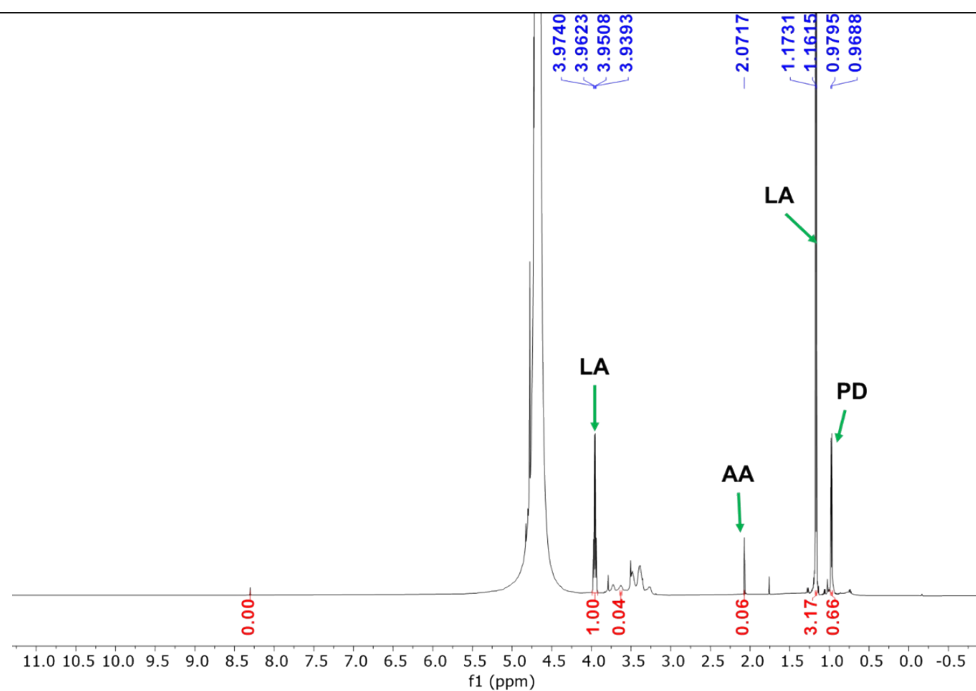
**Fig. S57**  $^1\text{H}$  NMR spectra of **Gly** to **LA** at 0.03 mol% of **Ru-1** at 298 K in  $\text{D}_2\text{O}$ .



**Fig. S58**  $^1\text{H}$  NMR spectra of **Gly** to **LA** at 0.05 mol% of **Ru-1** at 298 K in  $\text{D}_2\text{O}$ .

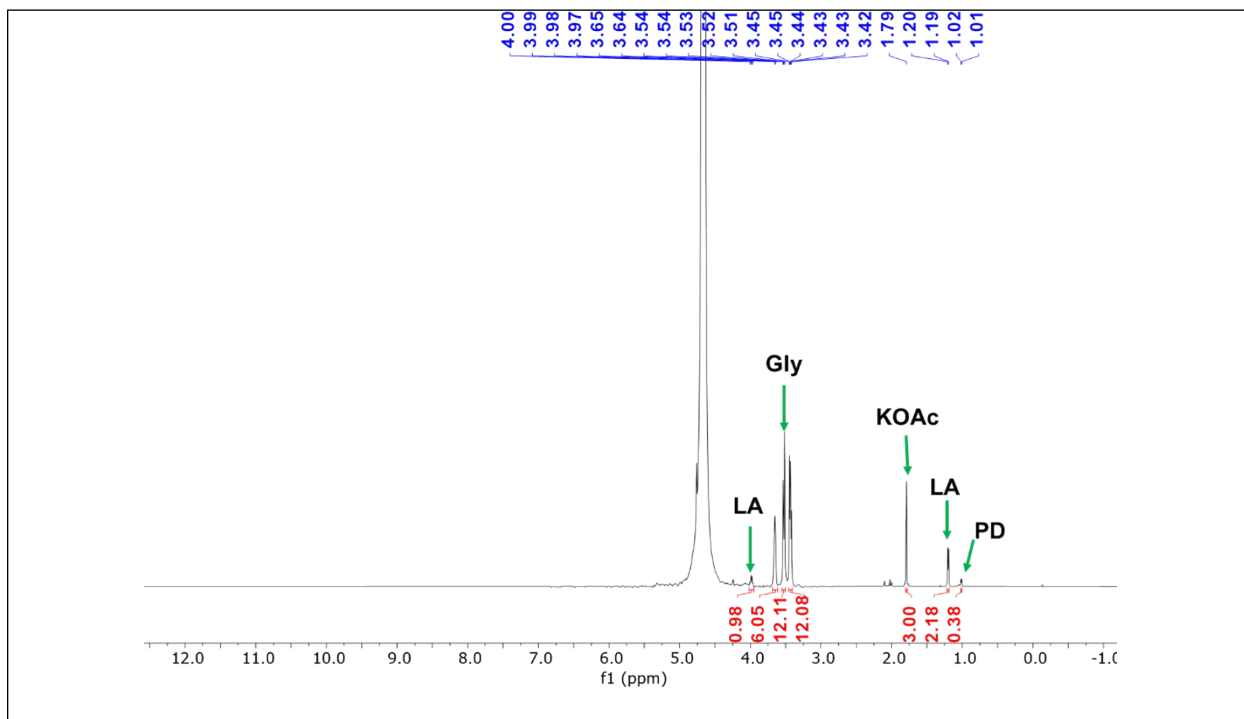


**Fig. S59**  $^1\text{H}$  NMR spectra of **Gly** to **LA** at 0.07 mol% of **Ru-1** at 298 K in  $\text{D}_2\text{O}$ .

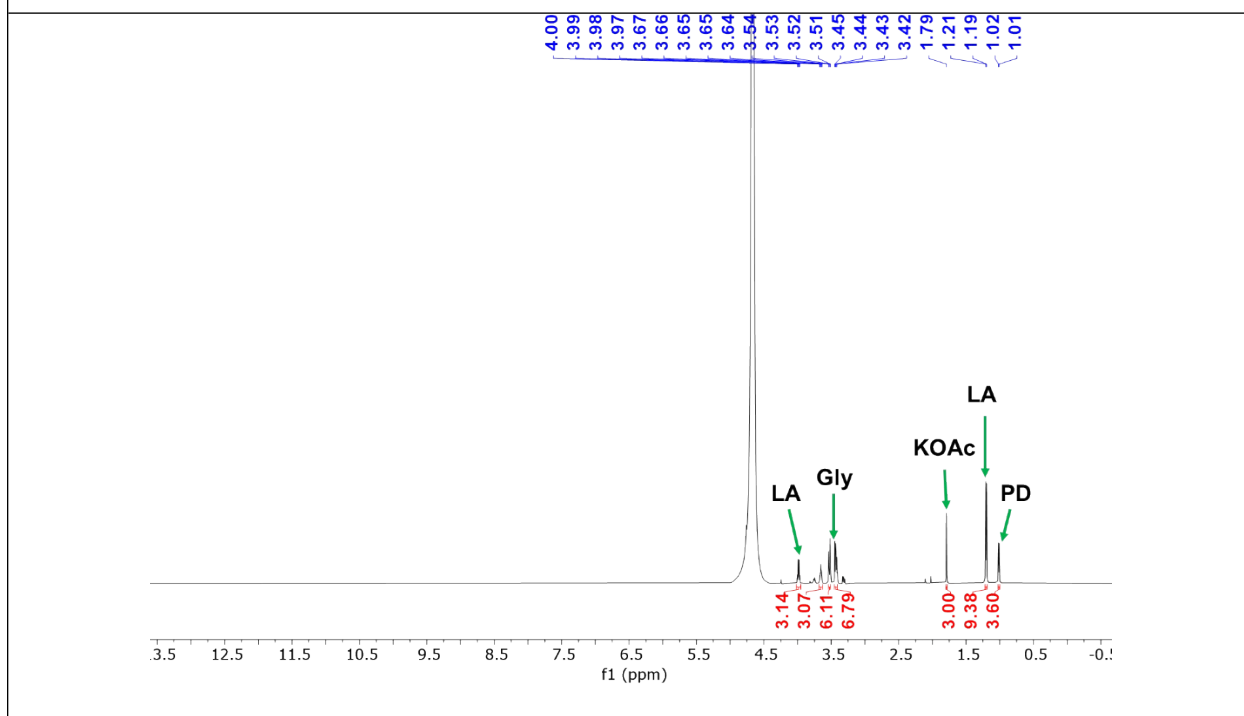


**Fig. S60**  $^1\text{H}$  NMR spectra of **Gly** to **LA** at 0.09 mol% of **Ru-1** at 298 K in  $\text{D}_2\text{O}$ .

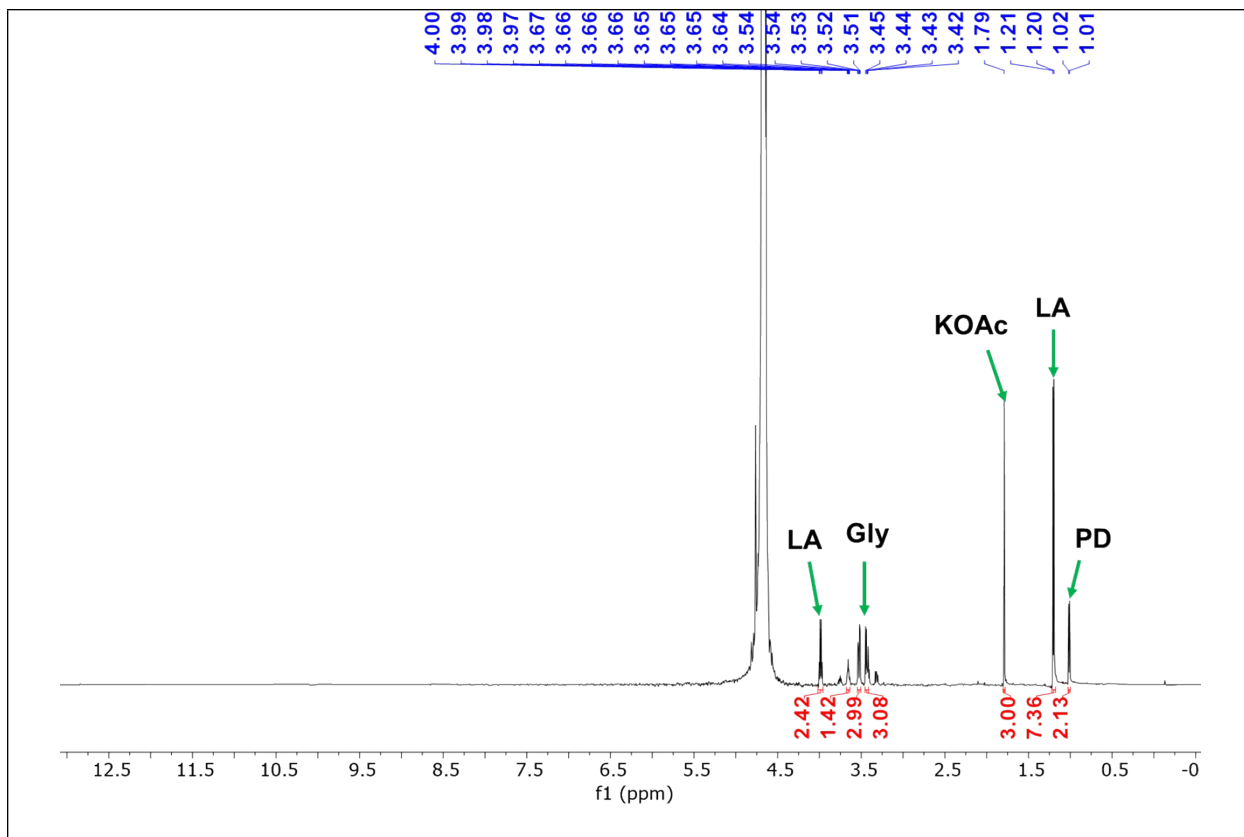
### 3.3 NaOH mmol Optimization



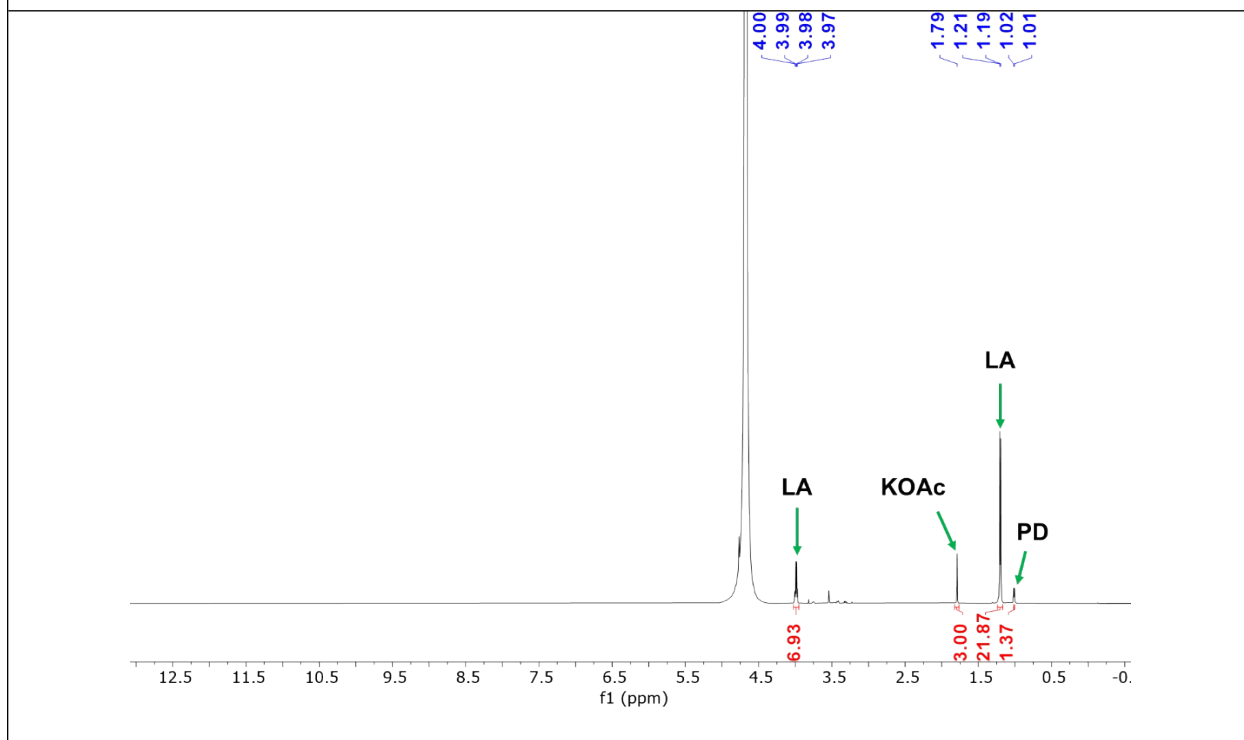
**Fig. S61** <sup>1</sup>H NMR spectra of **Gly** to **LA** at 1 mmol of NaOH at 298 K in D<sub>2</sub>O.



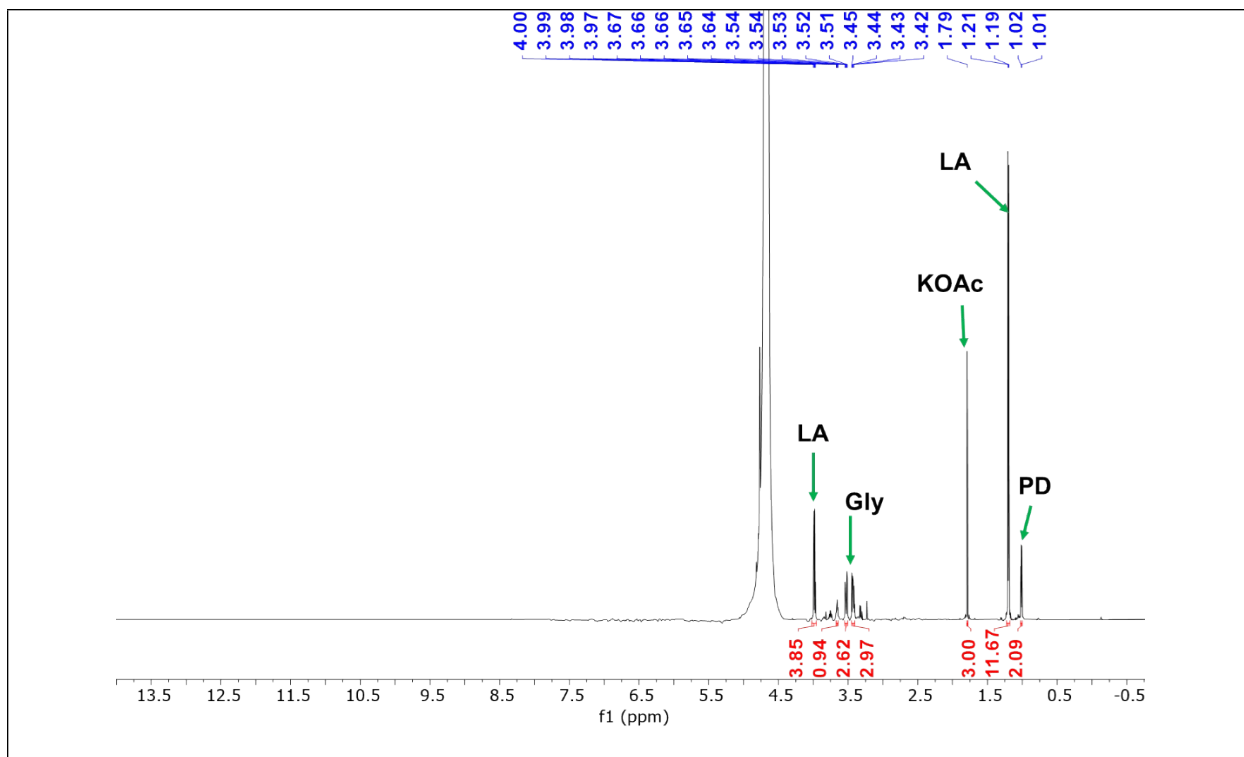
**Fig. S62** <sup>1</sup>H NMR spectra of **Gly** to **LA** at 3 mmol of NaOH at 298 K in D<sub>2</sub>O.



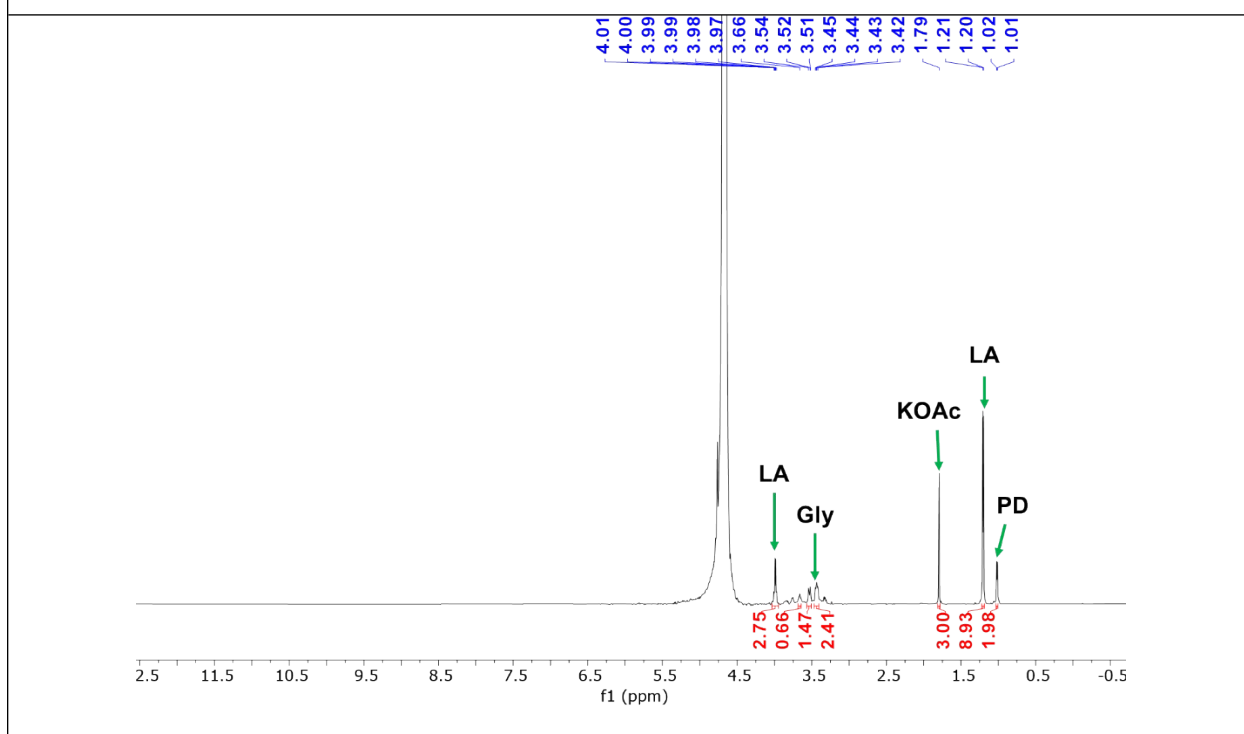
**Fig. S63**  $^1\text{H}$  NMR spectra of **Gly** to **LA** at 5 mmol of NaOH at 298 K in  $\text{D}_2\text{O}$ .



**Fig. S64**  $^1\text{H}$  NMR spectra of **Gly** to **LA** at 7 mmol of NaOH at 298 K in  $\text{D}_2\text{O}$ .

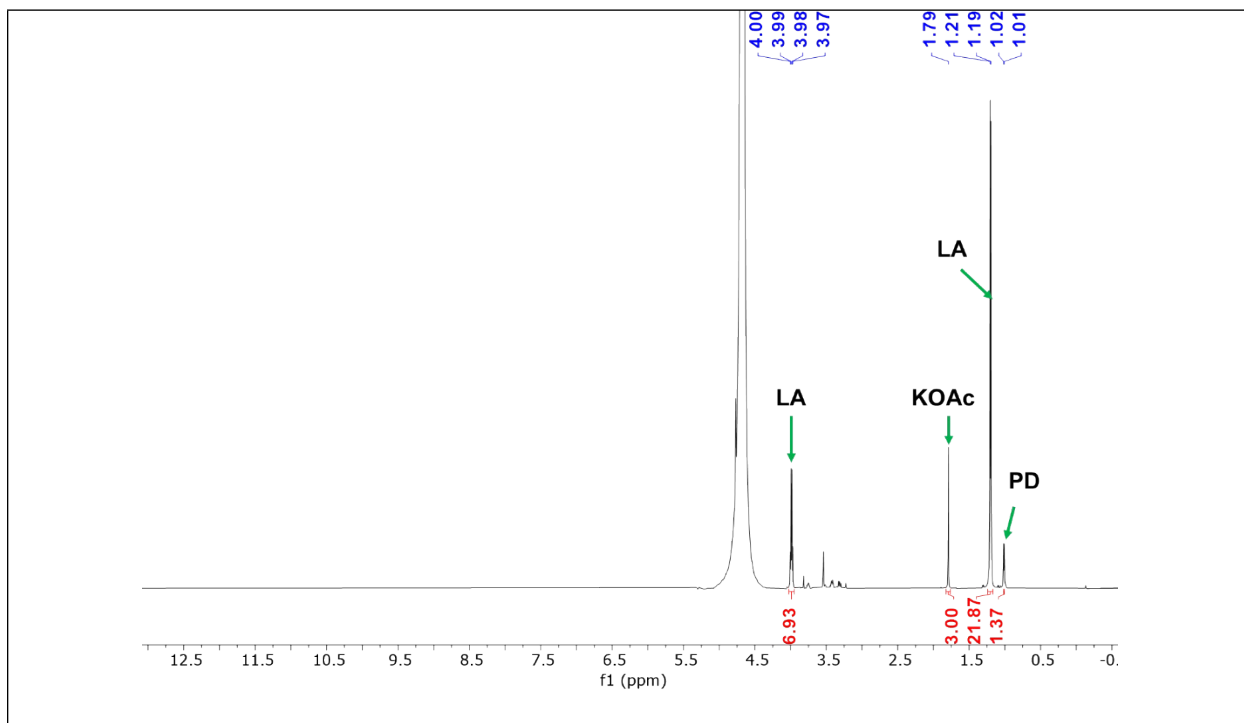


**Fig. S65**  $^1\text{H}$  NMR spectra of **Gly** to **LA** at 9 mmol of NaOH at 298 K in  $\text{D}_2\text{O}$ .

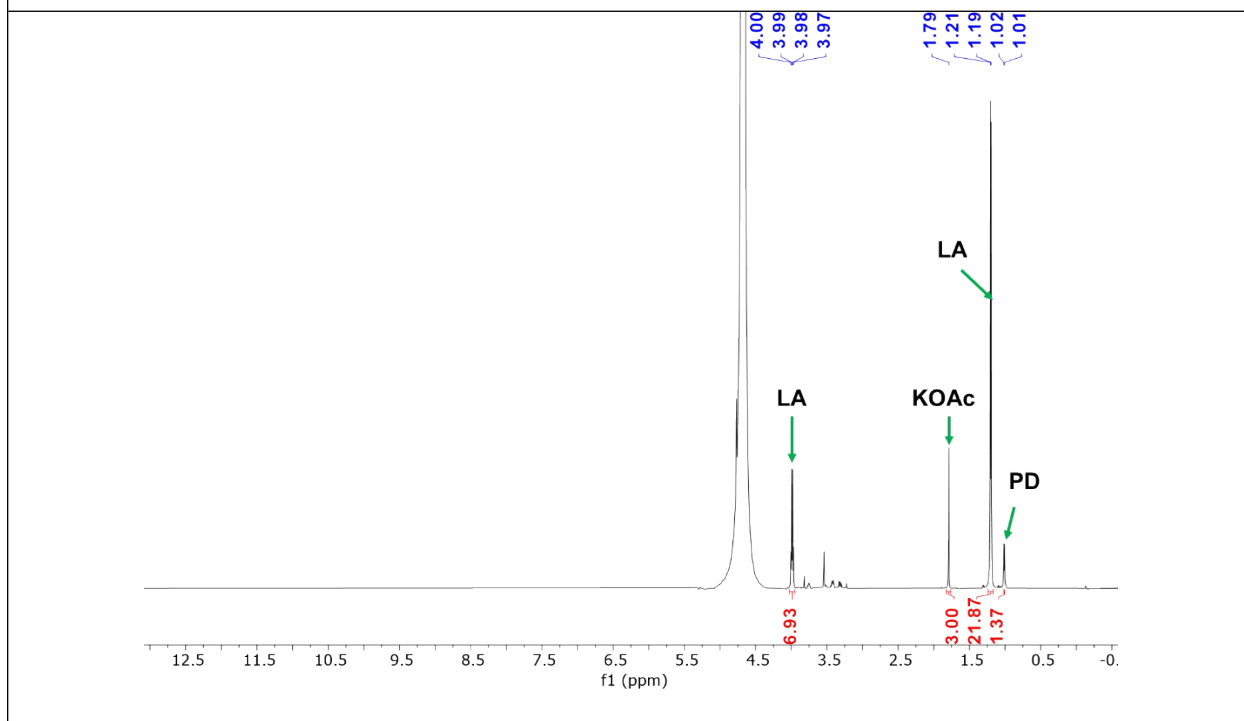


**Fig. S66**  $^1\text{H}$  NMR spectra of **Gly** to **LA** at 11 mmol of NaOH at 298 K in  $\text{D}_2\text{O}$ .

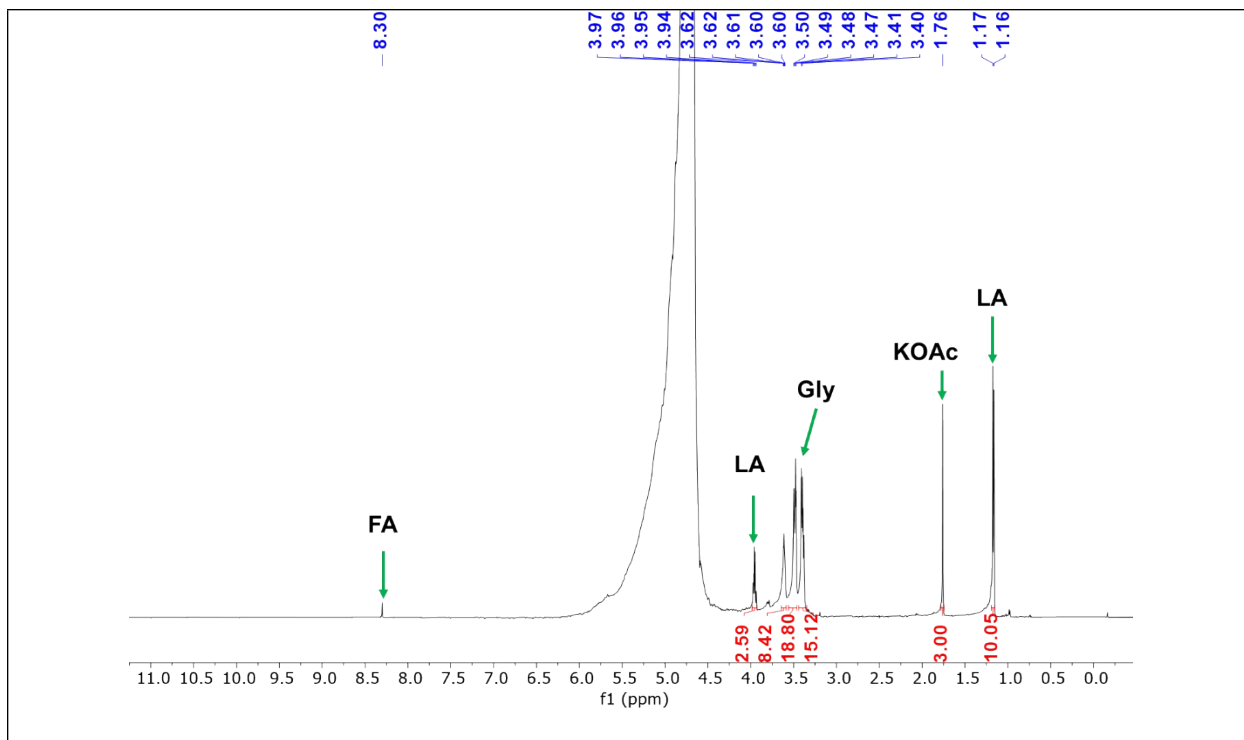
### 3.4 Solvent Screening



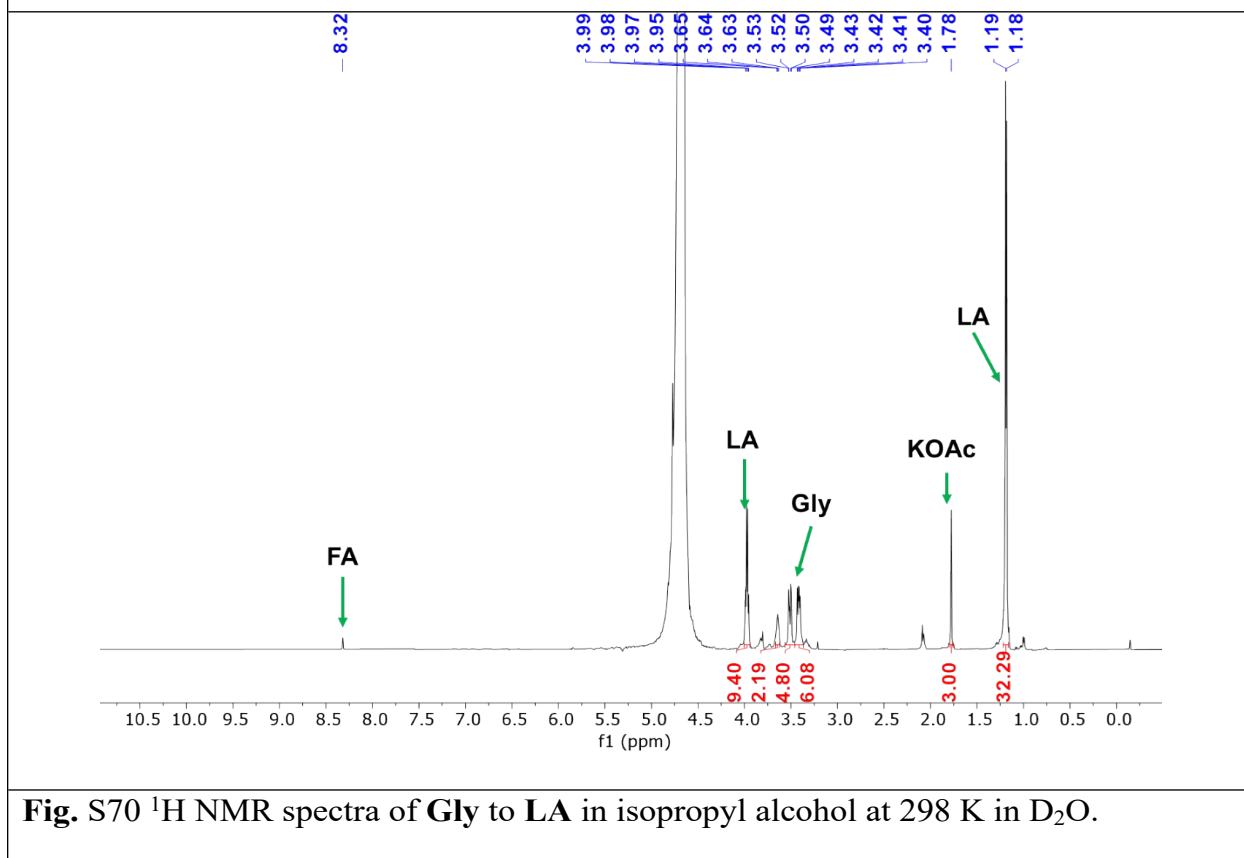
**Fig. S67** <sup>1</sup>H NMR spectra of **Gly** to **LA** in H<sub>2</sub>O at 298 K in D<sub>2</sub>O.



**Fig. S68** <sup>1</sup>H NMR spectra of **Gly** to **LA** in methanol at 298 K in D<sub>2</sub>O.



**Fig. S69**  $^1\text{H}$  NMR spectra of **Gly** to **LA** in ethanol at 298 K in  $\text{D}_2\text{O}$ .



**Fig. S70**  $^1\text{H}$  NMR spectra of **Gly** to **LA** in isopropyl alcohol at 298 K in  $\text{D}_2\text{O}$ .

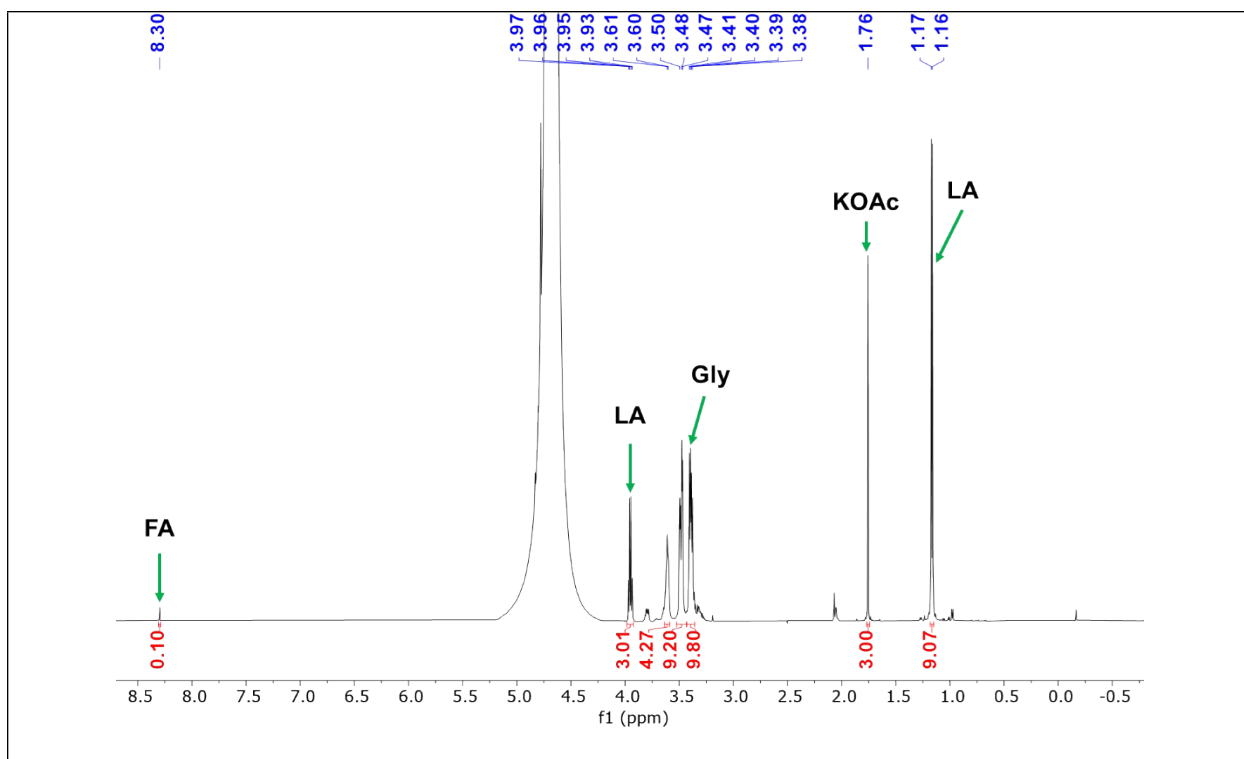


Fig. S71 <sup>1</sup>H NMR spectra of Gly to LA in acetone at 298 K in D<sub>2</sub>O.

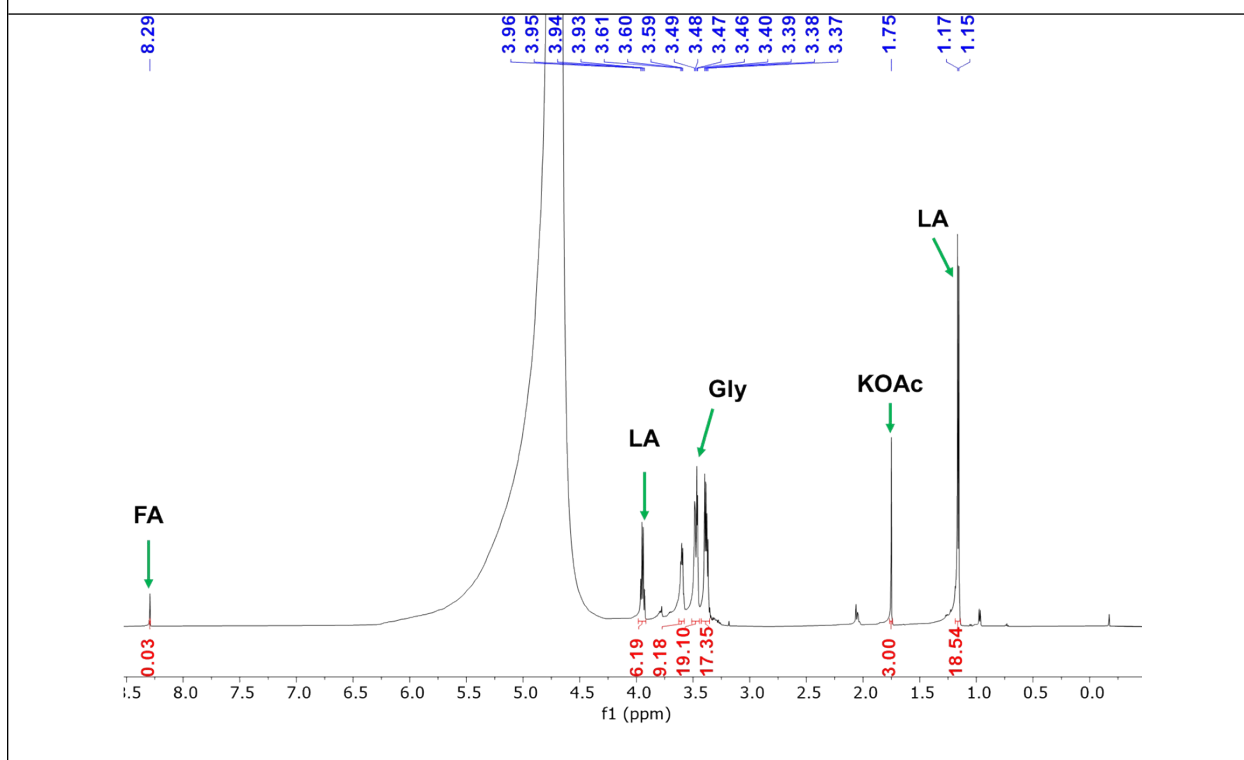
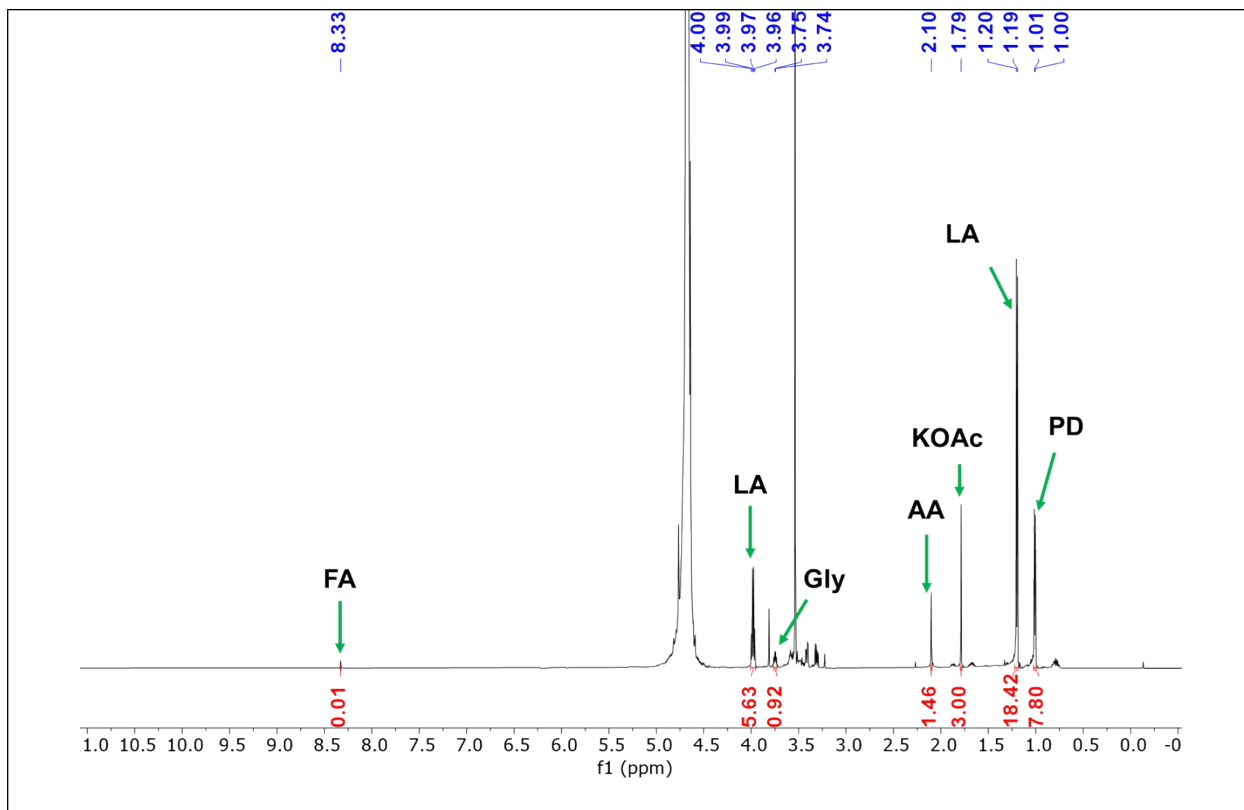
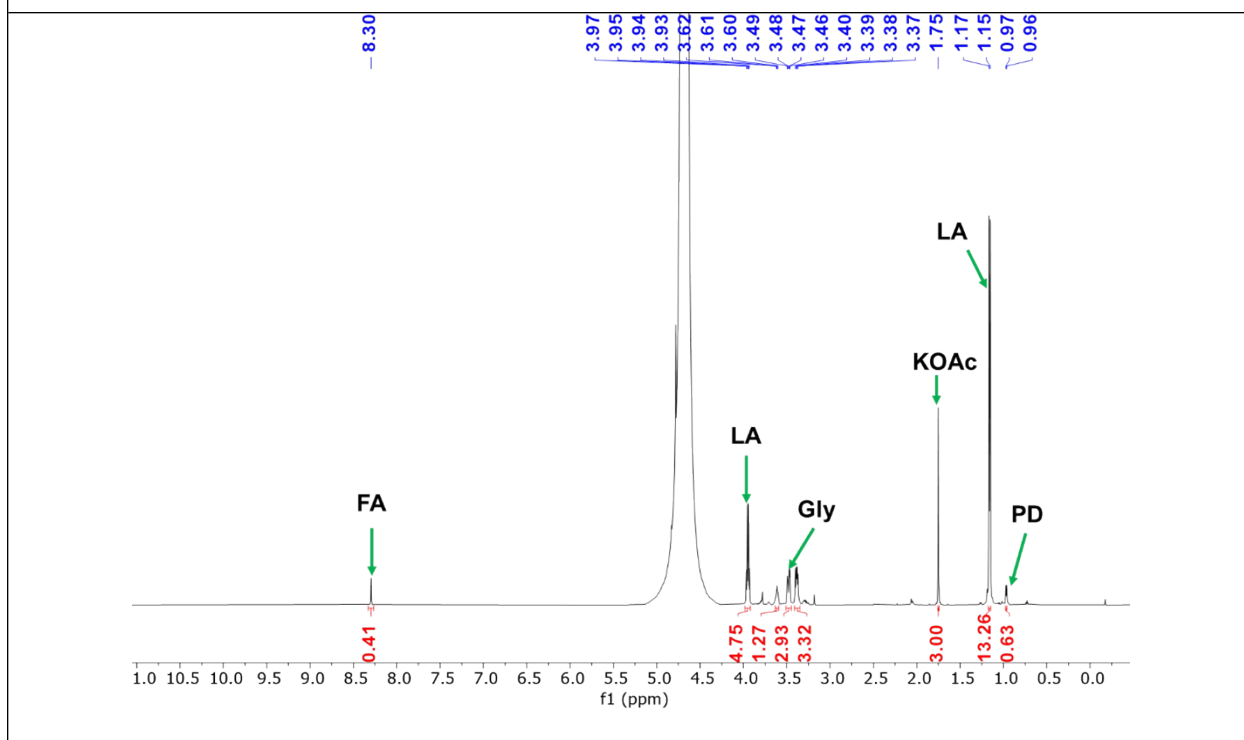


Fig. S72 <sup>1</sup>H NMR spectra of Gly to LA in 1,4-dioxane at 298 K in D<sub>2</sub>O.

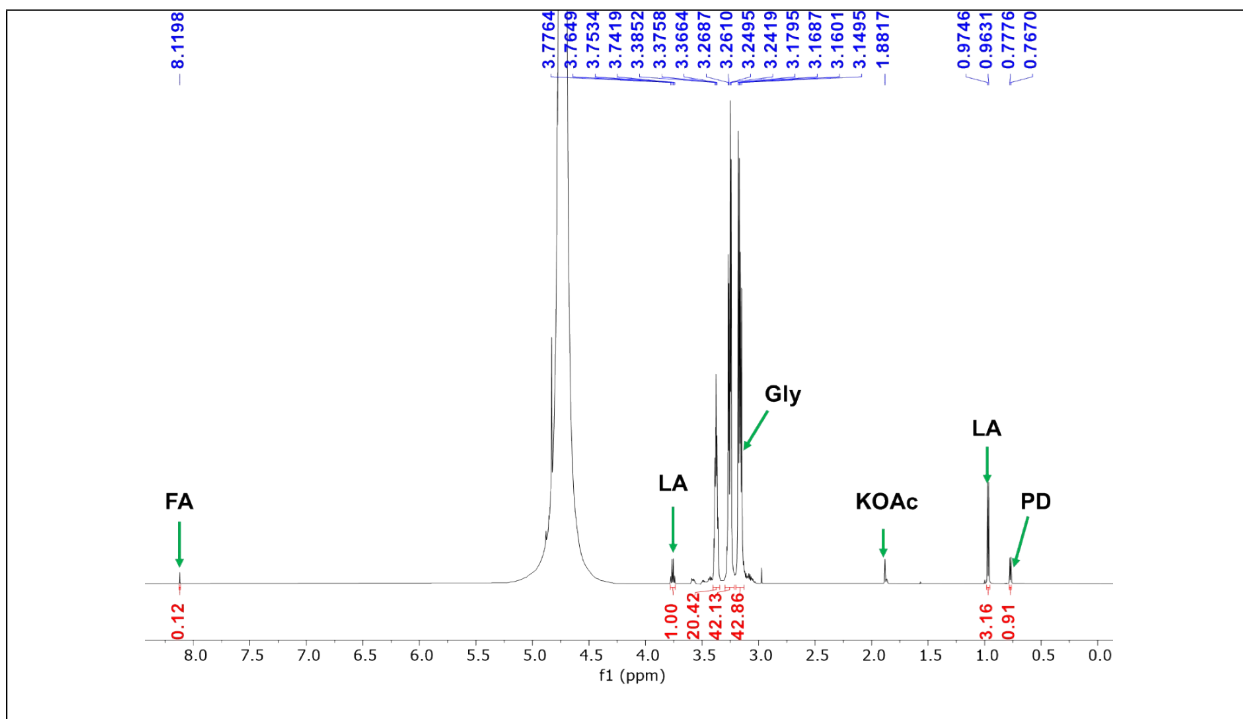


**Fig. S73**  $^1\text{H}$  NMR spectra of Gly to LA in ethylene glycol at 298 K in  $\text{D}_2\text{O}$ .

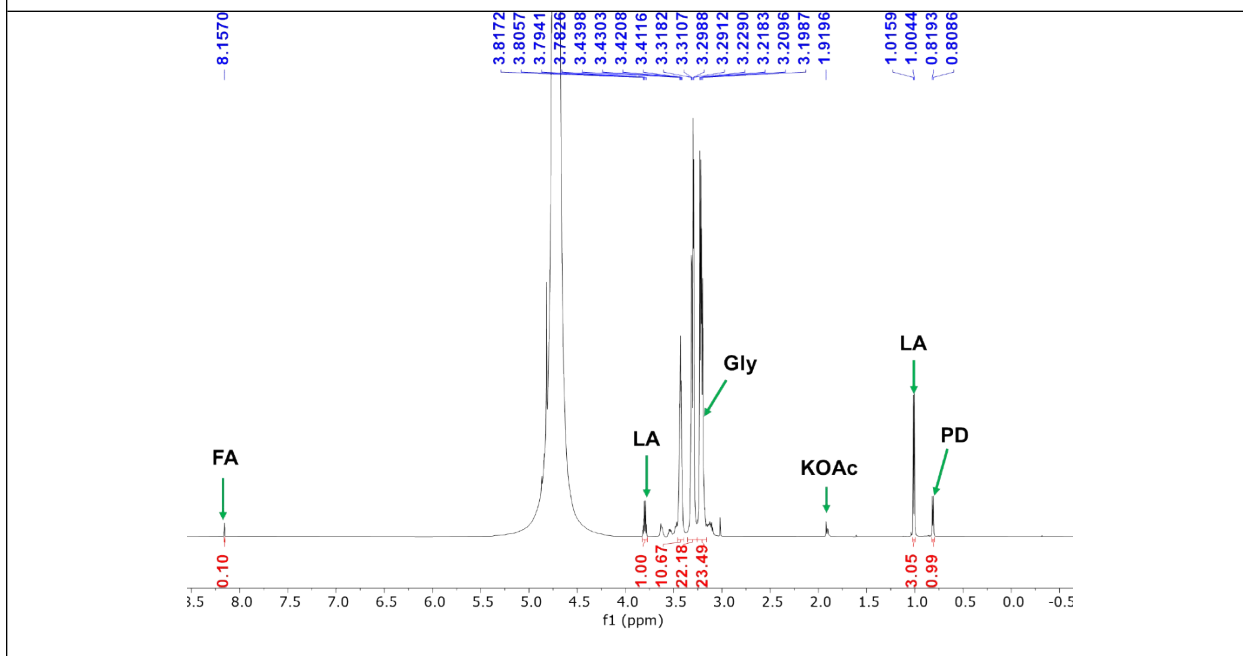


**Fig. S74**  $^1\text{H}$  NMR spectra of Gly to LA neat at 298 K in  $\text{D}_2\text{O}$ .

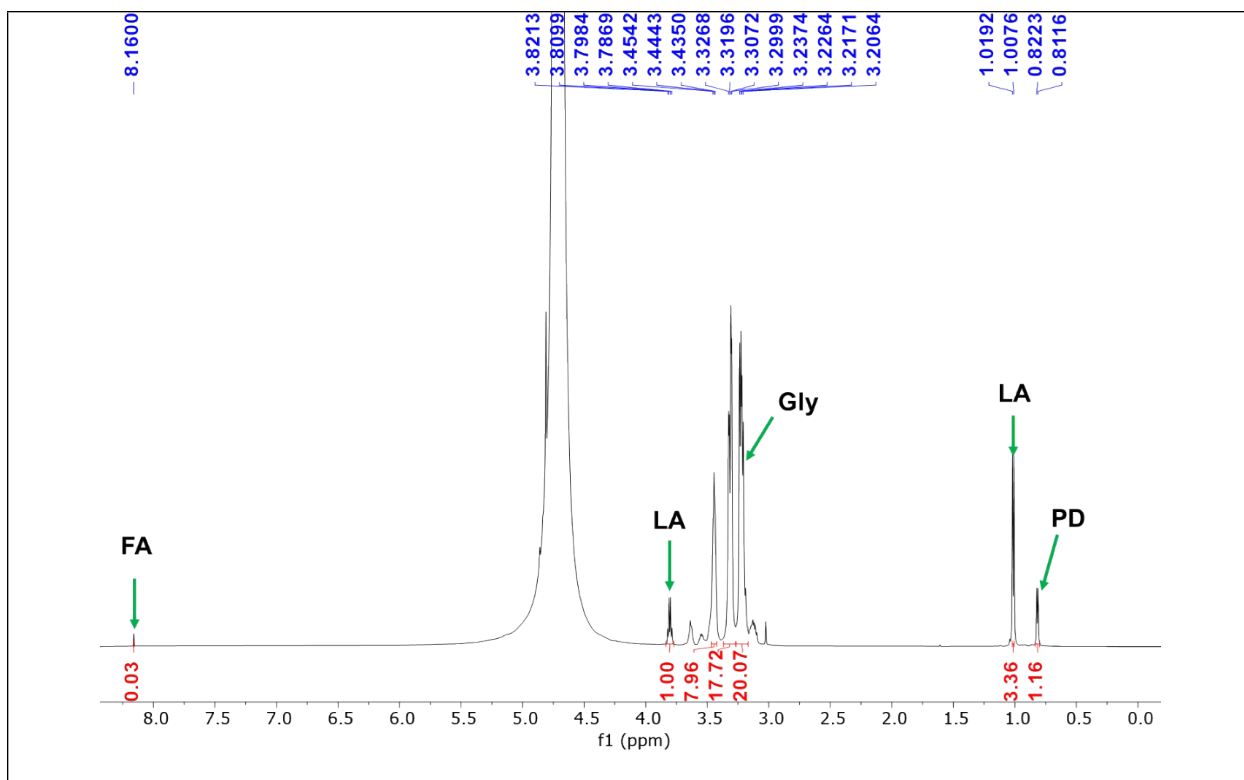
### 3.5 Time Optimization



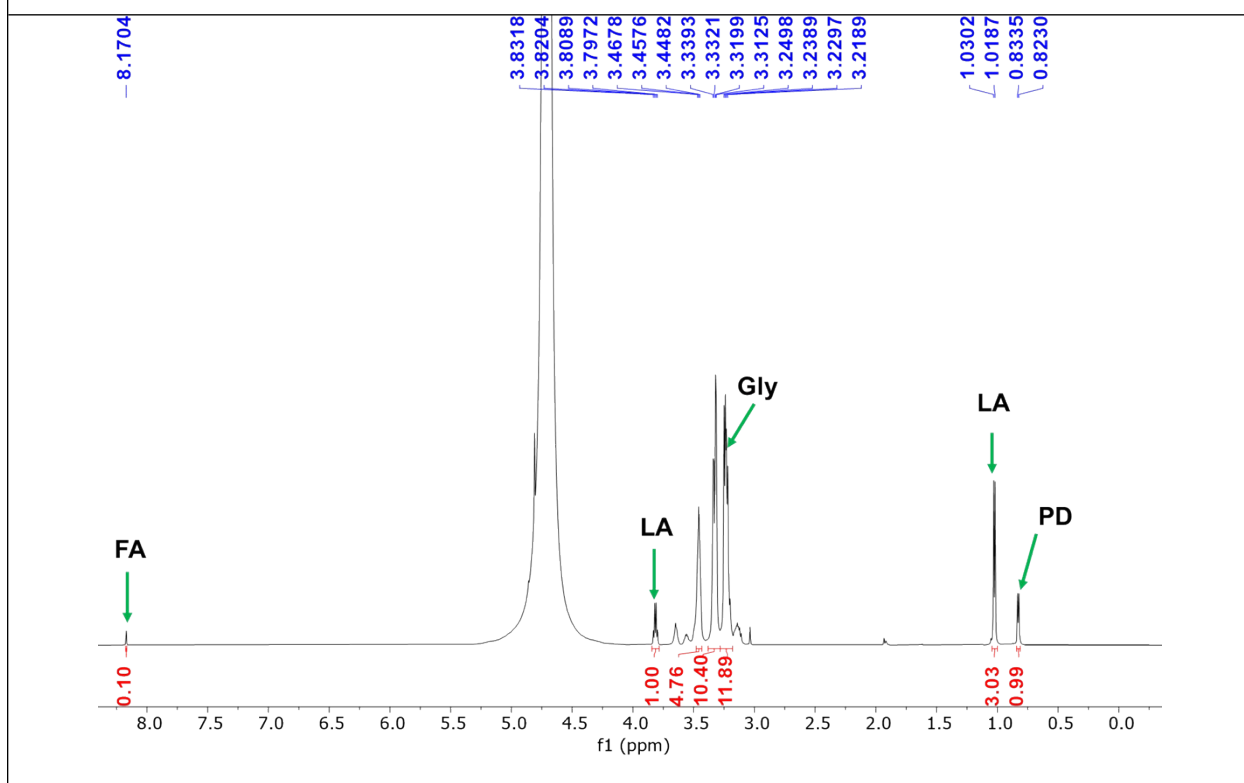
**Fig. S75**  $^1\text{H}$  NMR spectra of Gly to LA after 1h at 298 K in  $\text{D}_2\text{O}$ .



**Fig. S76**  $^1\text{H}$  NMR spectra of Gly to LA after 2h at 298 K in  $\text{D}_2\text{O}$ .



**Fig. S77**  $^1\text{H}$  NMR spectra of Gly to LA after 3h at 298 K in  $\text{D}_2\text{O}$ .



**Fig. S78**  $^1\text{H}$  NMR spectra of Gly to LA after 4h at 298 K in  $\text{D}_2\text{O}$ .

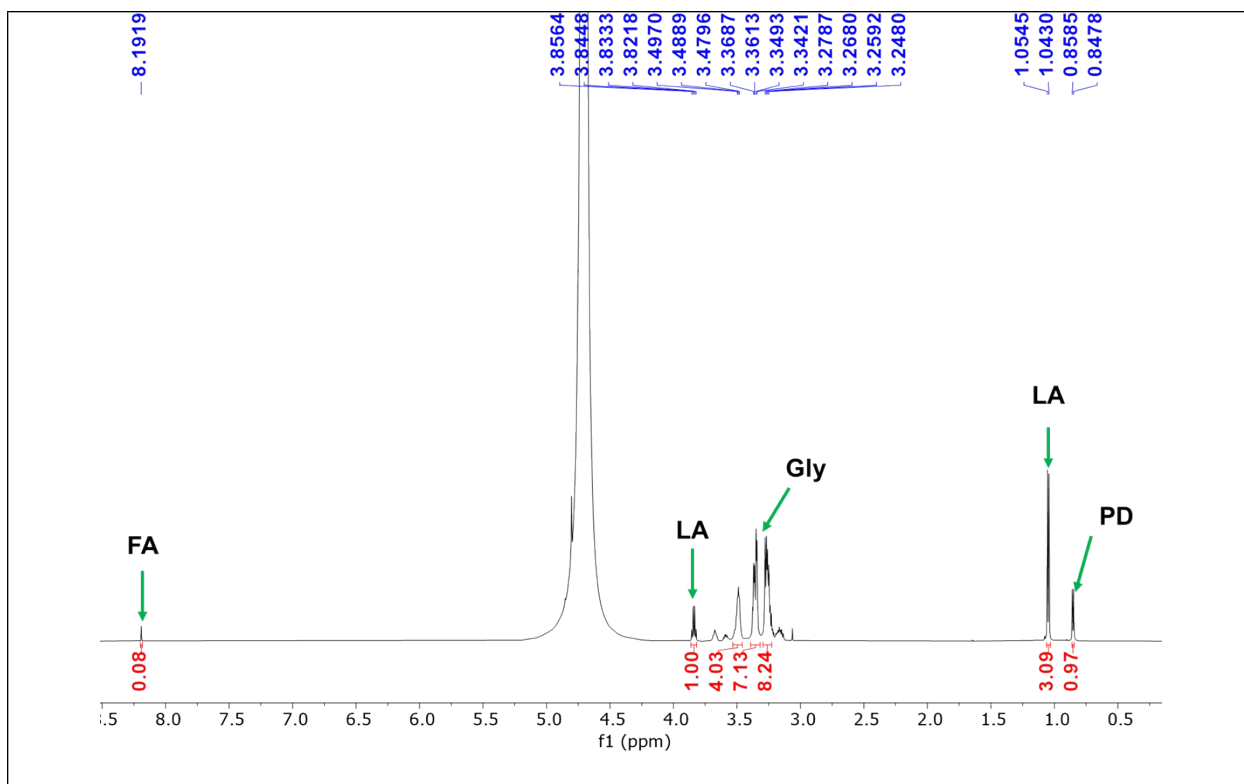


Fig. S79  $^1\text{H}$  NMR spectra of Gly to LA after 6h at 298 K in  $\text{D}_2\text{O}$ .

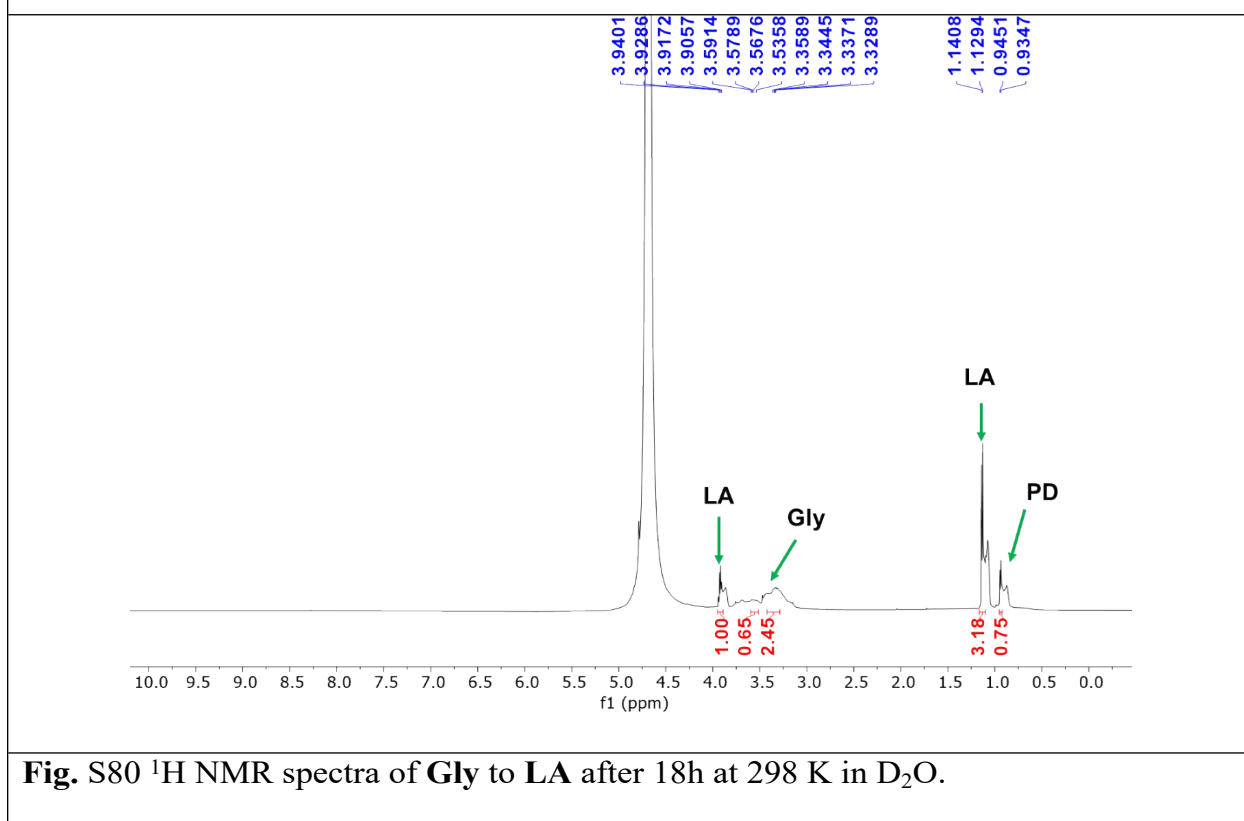


Fig. S80  $^1\text{H}$  NMR spectra of Gly to LA after 18h at 298 K in  $\text{D}_2\text{O}$ .

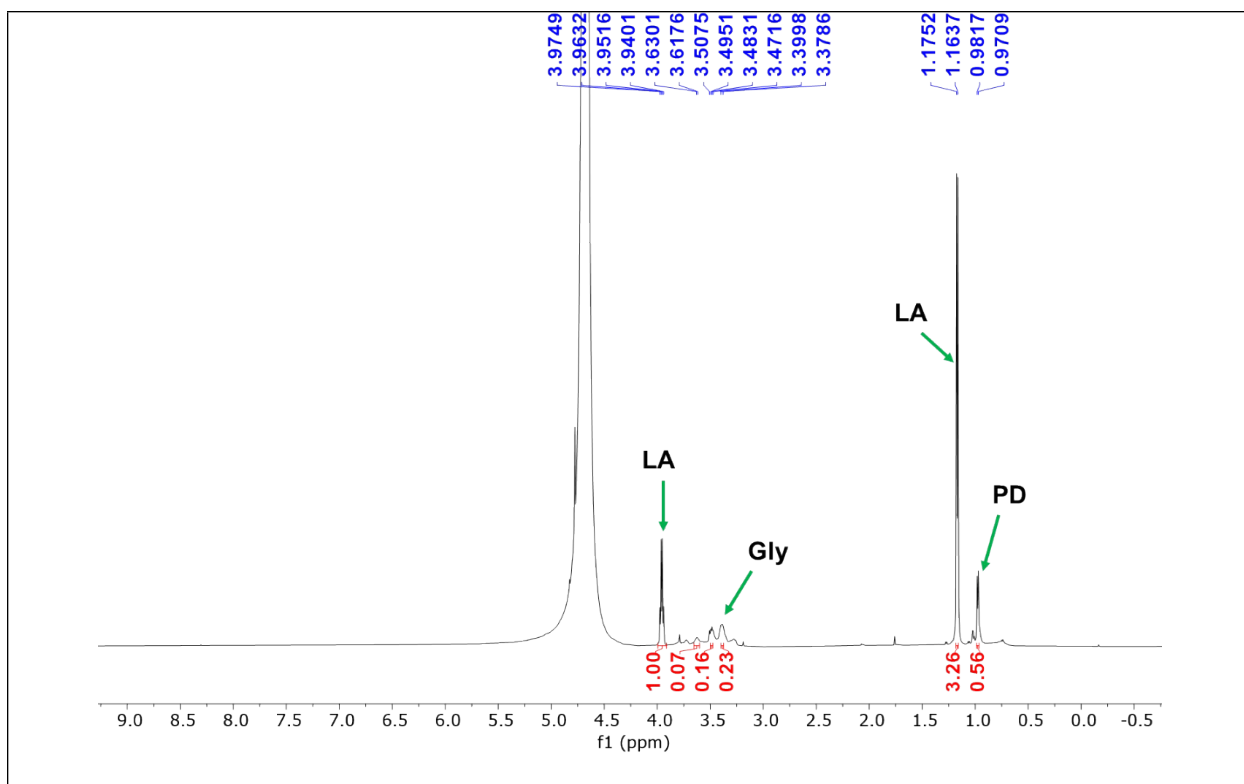


Fig. S81  $^1\text{H}$  NMR spectra of Gly to LA after 24h at 298 K in  $\text{D}_2\text{O}$ .

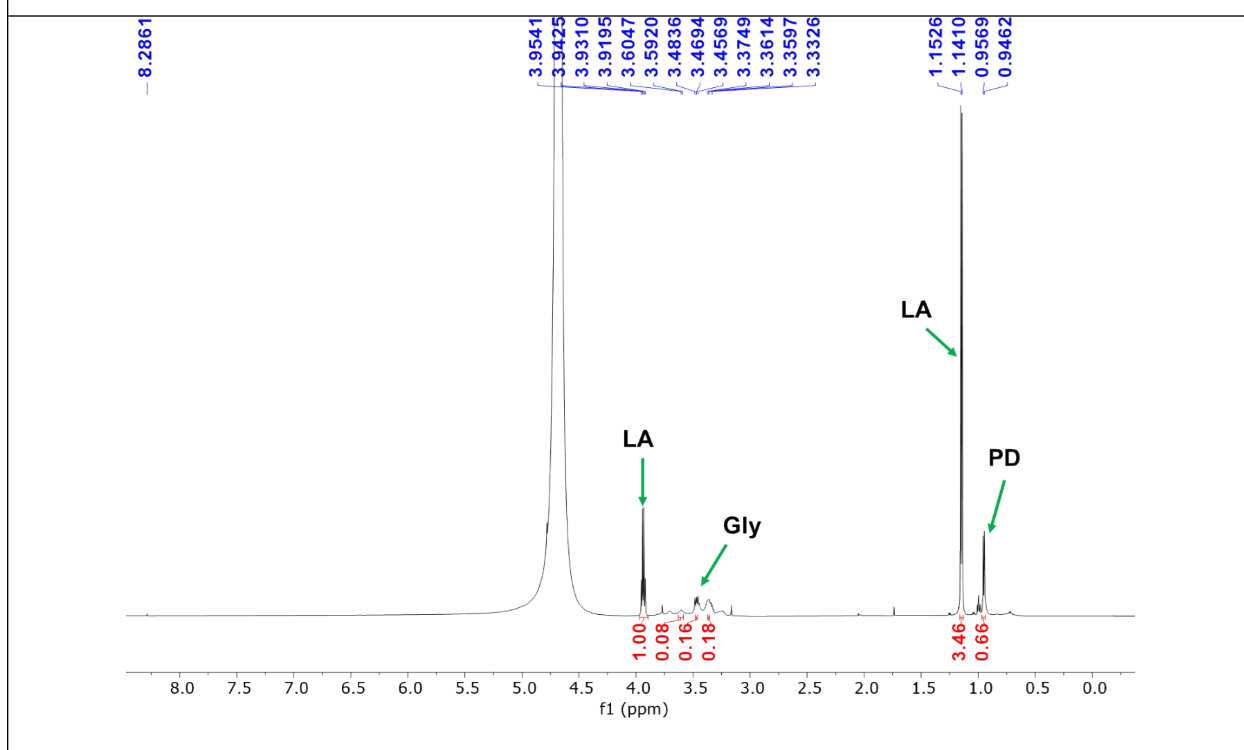


Fig. S82  $^1\text{H}$  NMR spectra of Gly to LA after 30h at 298 K in  $\text{D}_2\text{O}$ .

### 3.6 Temperature optimization

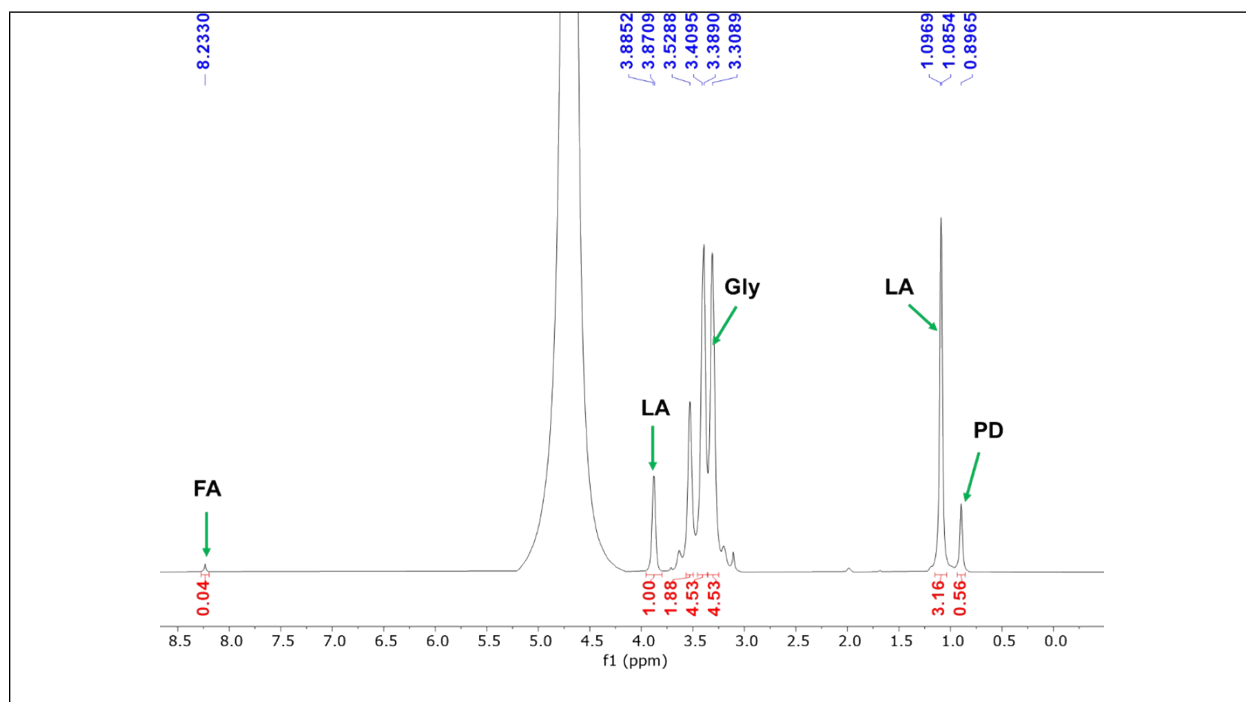


Fig. S83 <sup>1</sup>H NMR spectra of Gly to LA at 140°C at 298 K in D<sub>2</sub>O.

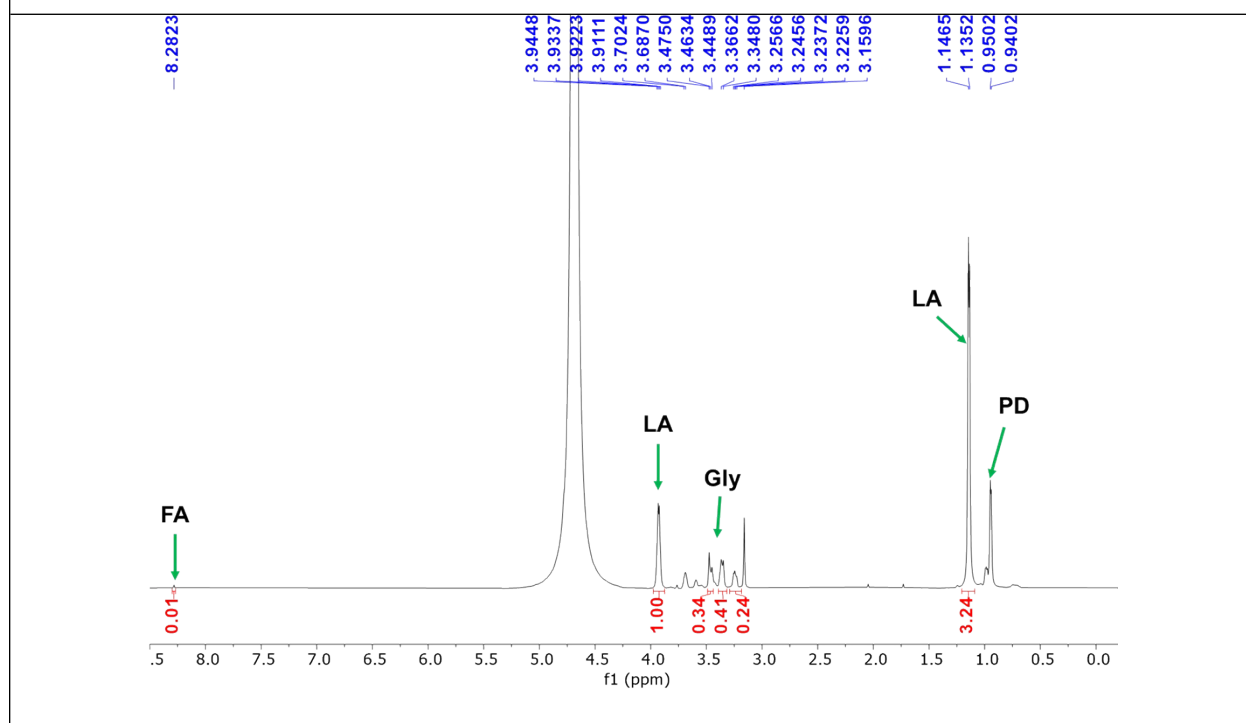
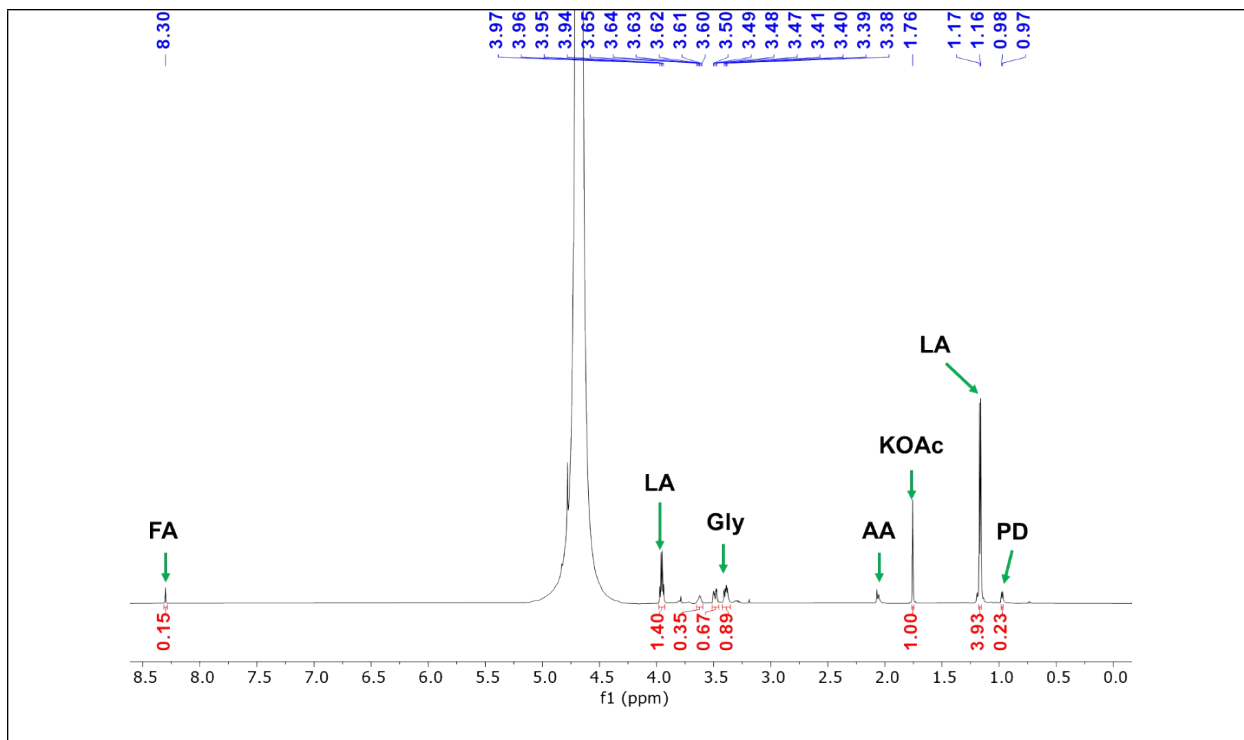
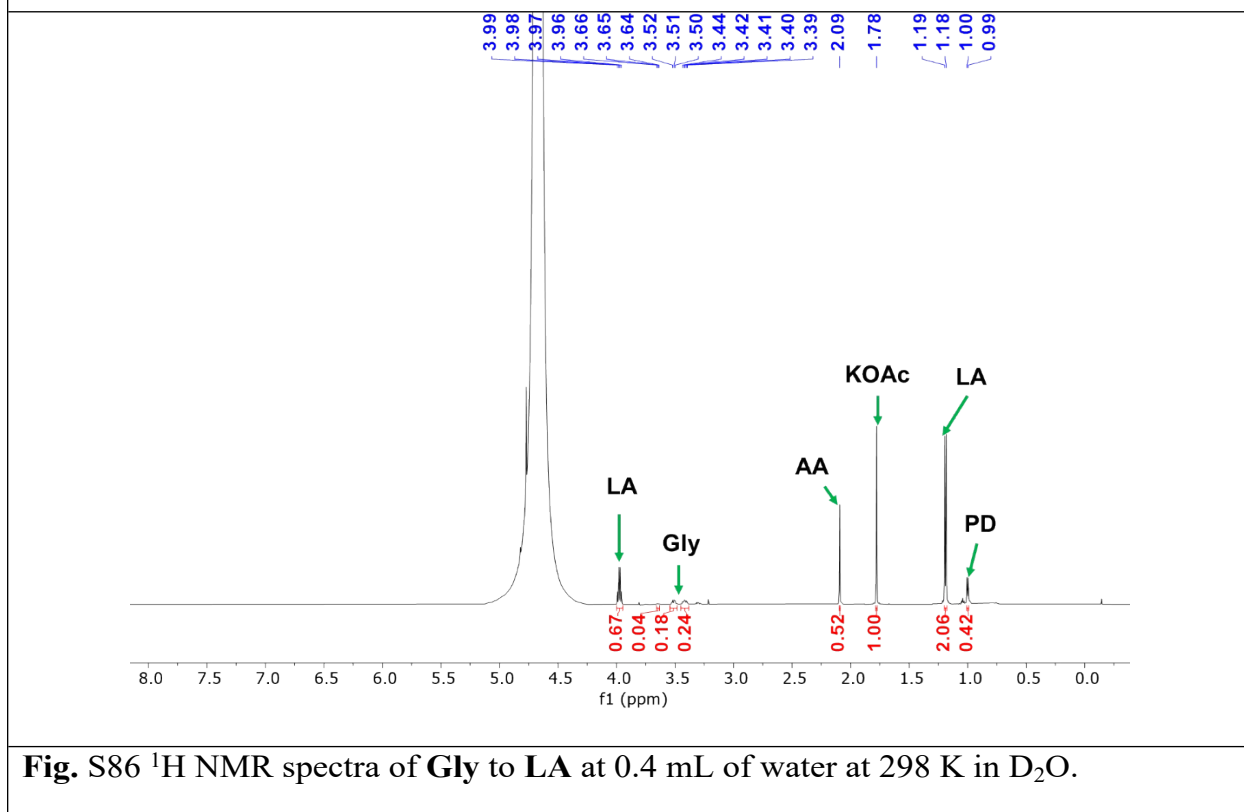


Fig. S84 <sup>1</sup>H NMR spectra of Gly to LA at 150°C at 298 K in D<sub>2</sub>O.

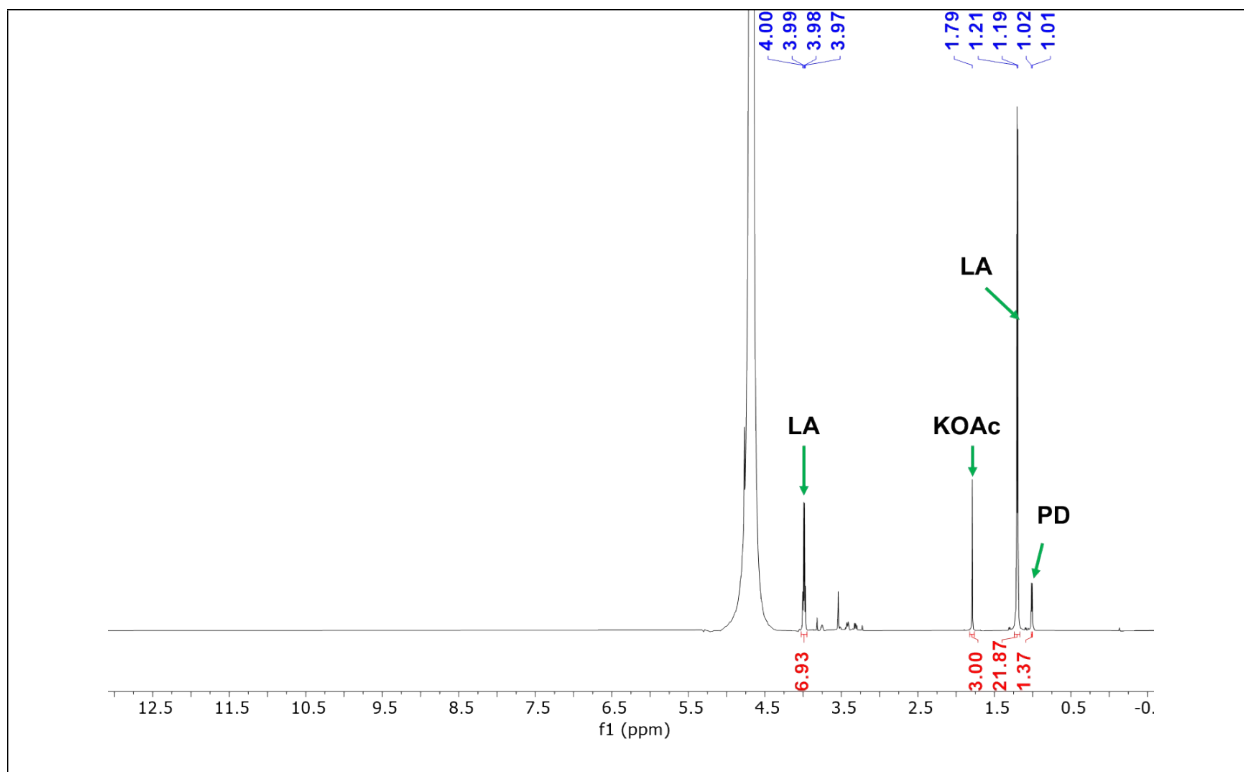
### 3.7 Water amount optimization



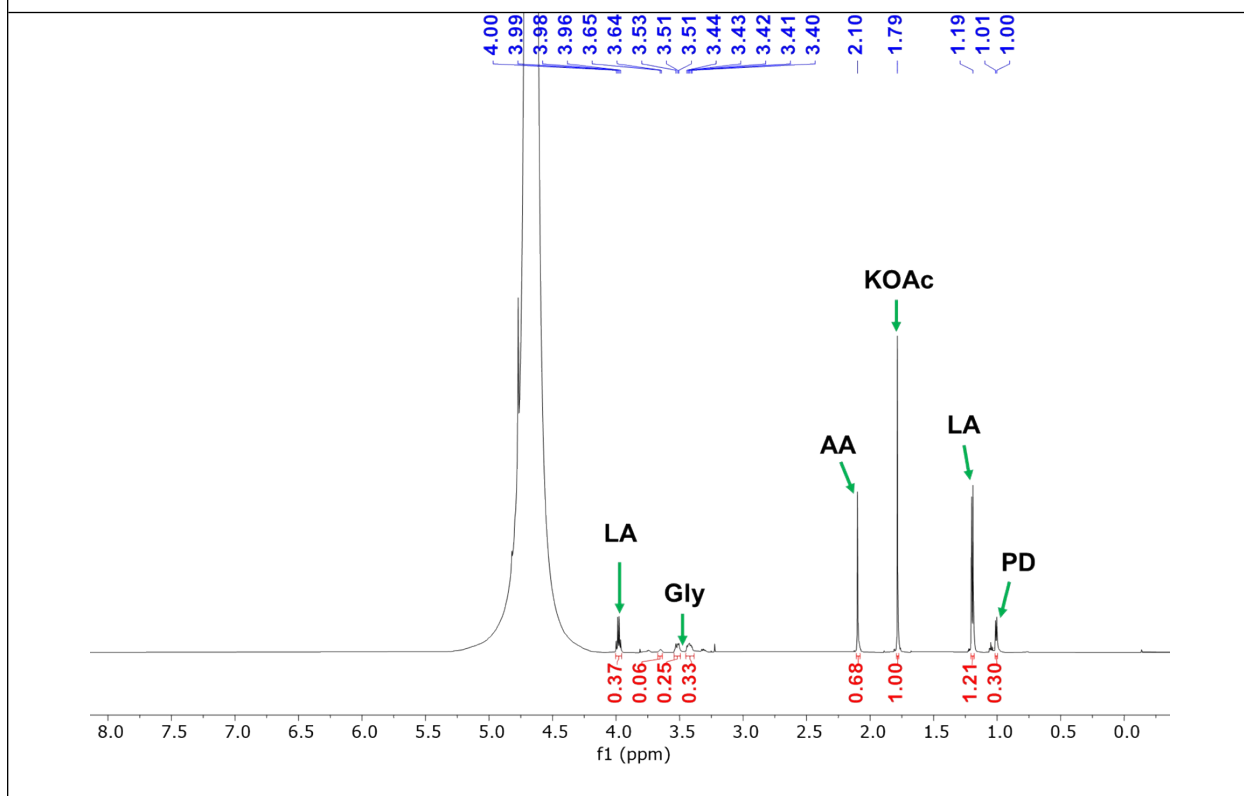
**Fig. S85**  $^1\text{H}$  NMR spectra of Gly to LA at 0.2 mL of water at 298 K in  $\text{D}_2\text{O}$ .



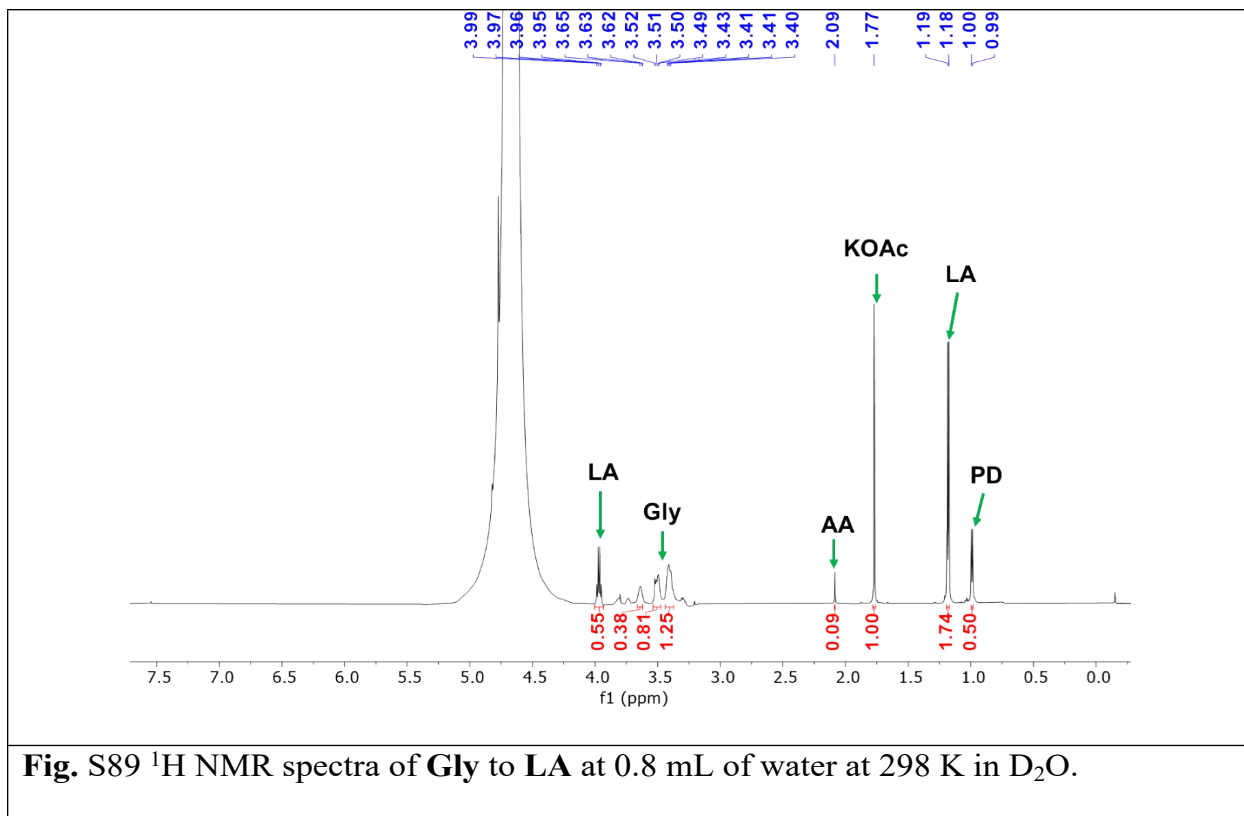
**Fig. S86**  $^1\text{H}$  NMR spectra of Gly to LA at 0.4 mL of water at 298 K in  $\text{D}_2\text{O}$ .



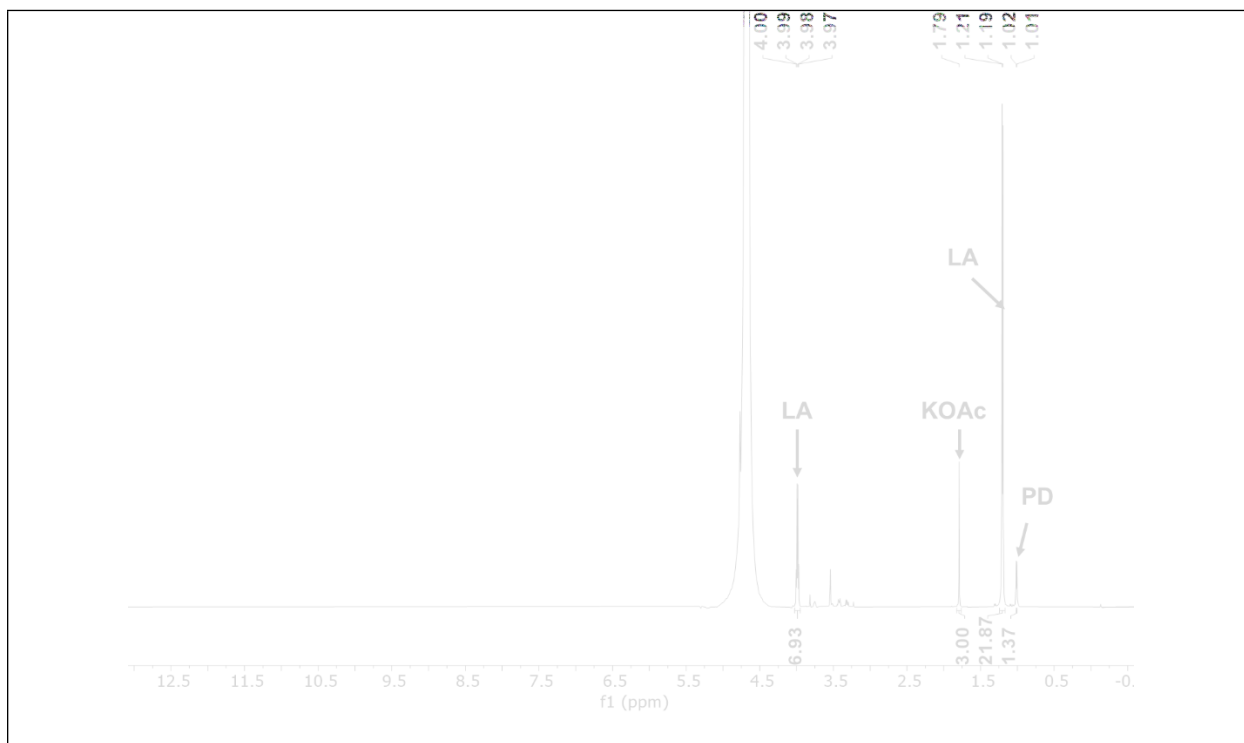
**Fig. S87**  $^1\text{H}$  NMR spectra of **Gly** to **LA** at 0.5 mL of water at 298 K in  $\text{D}_2\text{O}$ .



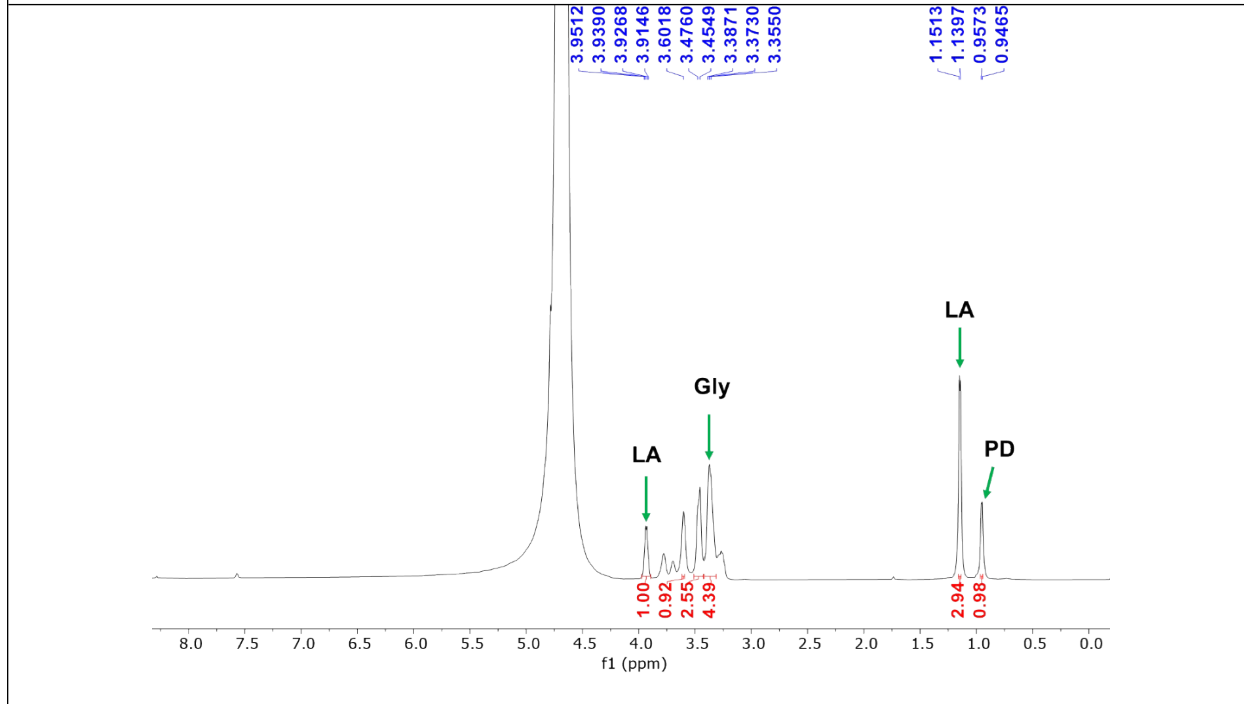
**Fig. S88**  $^1\text{H}$  NMR spectra of **Gly** to **LA** at 0.6 mL of water at 298 K in  $\text{D}_2\text{O}$ .



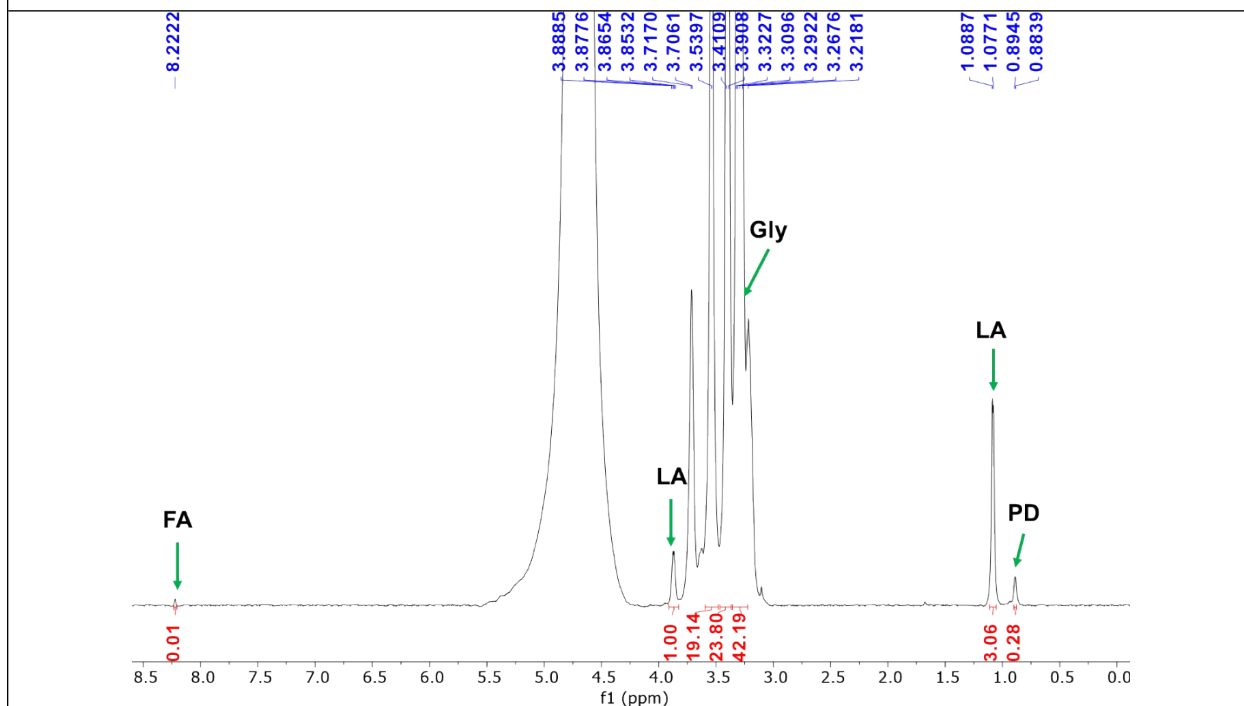
### 3.8 Catalyst Optimization



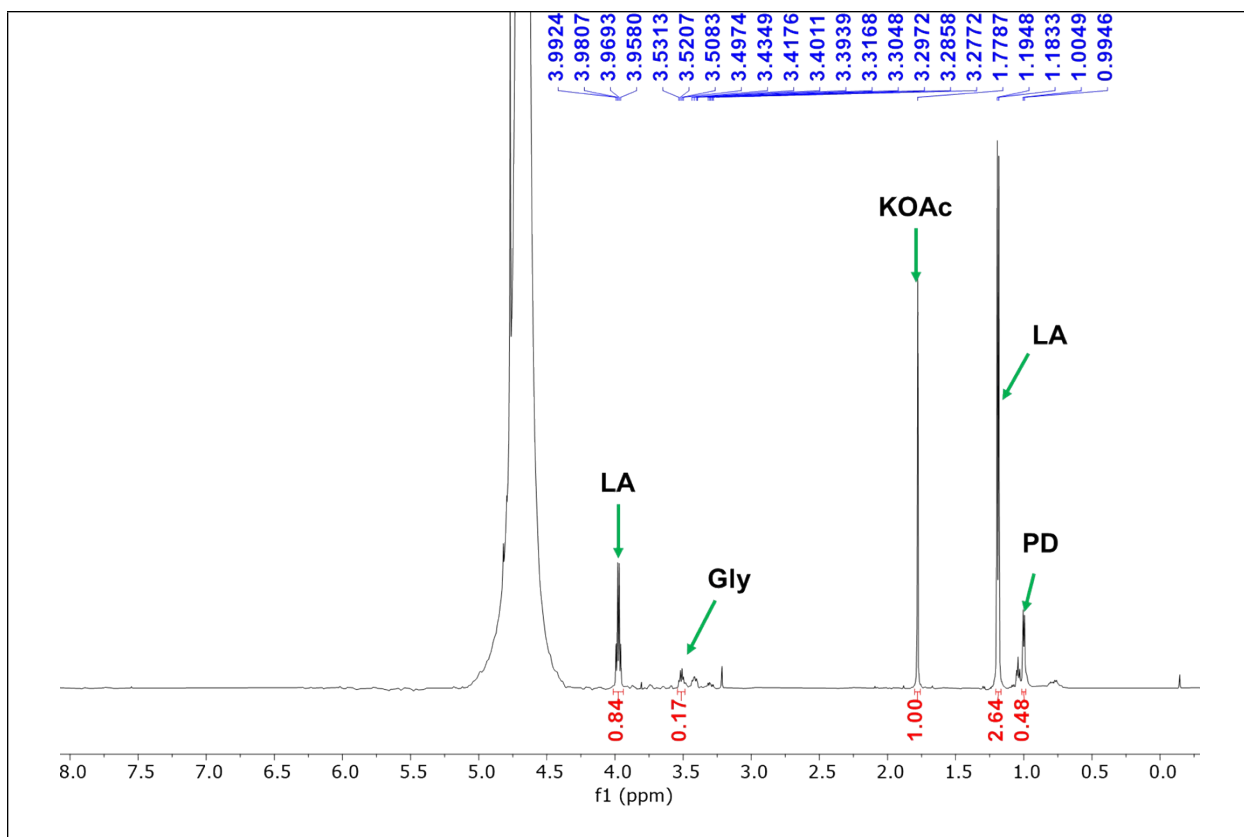
**Fig. S90**  $^1\text{H}$  NMR spectra of **Gly** to **LA** using **Ru-1** at 298 K in  $\text{D}_2\text{O}$ .



**Fig. S91**  $^1\text{H}$  NMR spectra of **Gly** to **LA** using **Ru-1N<sup>Me</sup>** at 298 K in  $\text{D}_2\text{O}$ .



**Fig. S92**  $^1\text{H}$  NMR spectra of **Gly** to **LA** using **Ru-2** at 298 K in  $\text{D}_2\text{O}$ .



**Fig. S93**  $^1\text{H}$  NMR spectra of **Gly** to **LA** using **Ru-3** at 298 K in  $\text{D}_2\text{O}$ .

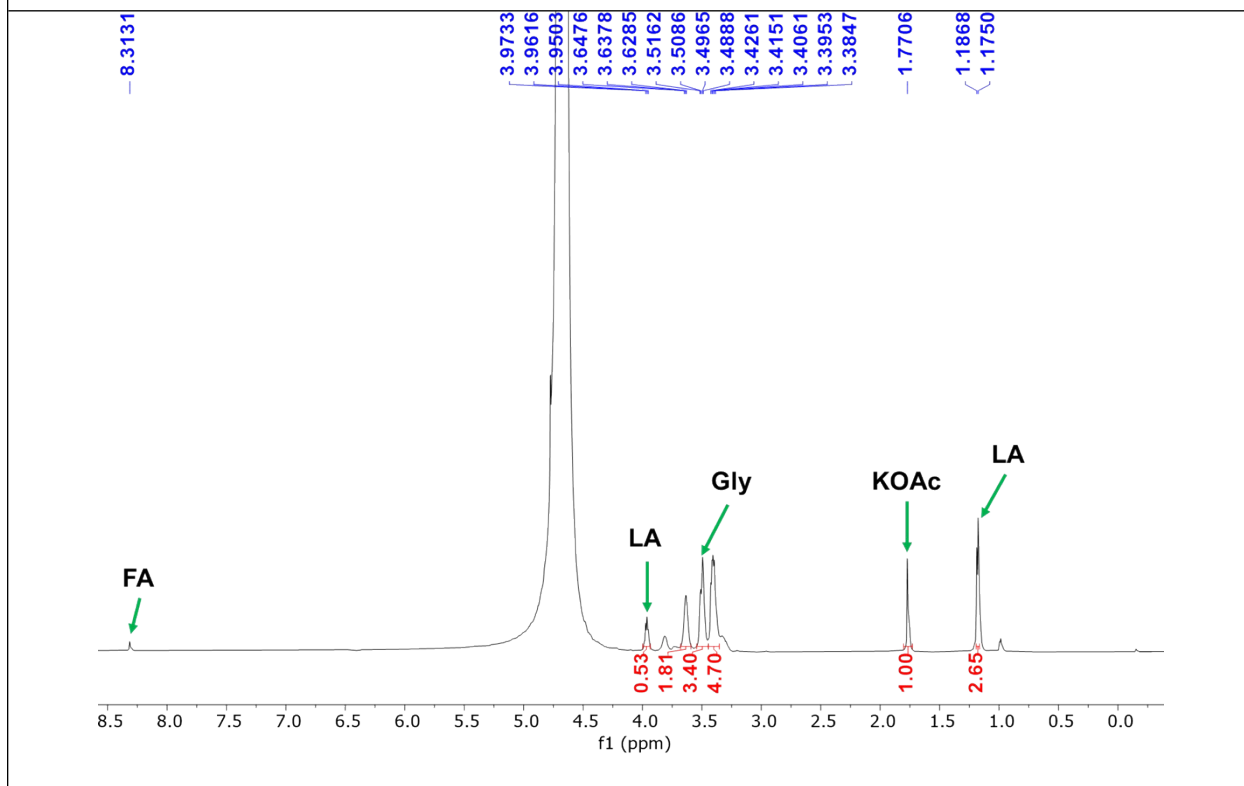


Fig. S94  $^1\text{H}$  NMR spectra of Gly to LA using Ru-3N<sup>Me</sup> at 298 K in D<sub>2</sub>O.

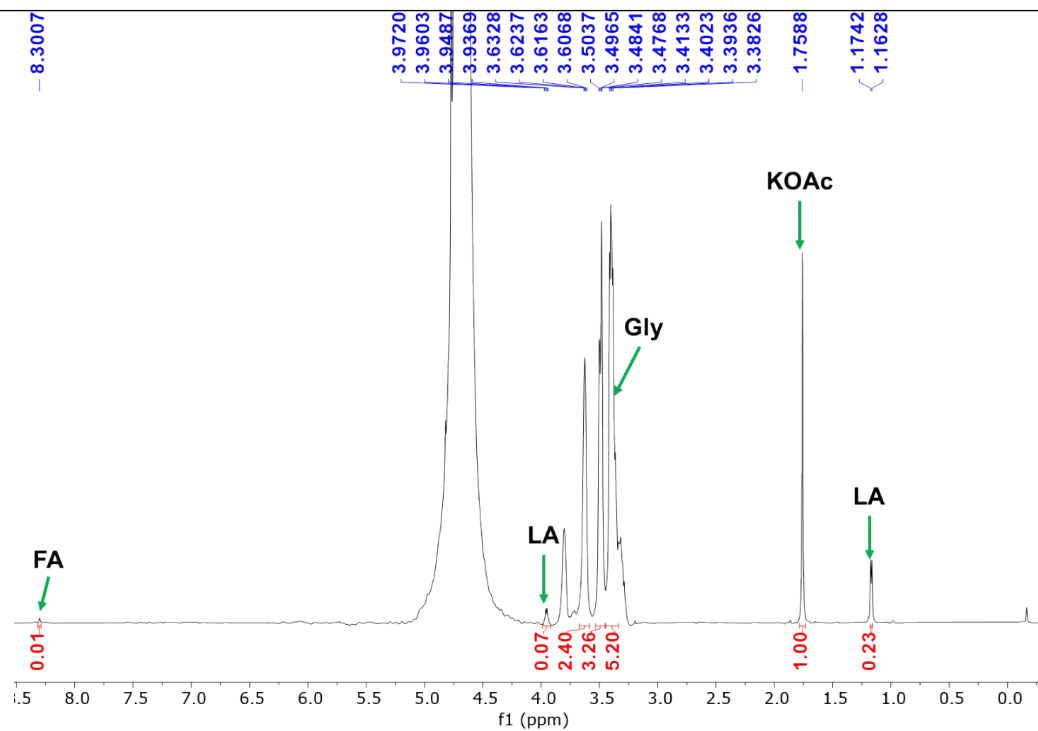


Fig. S95  $^1\text{H}$  NMR spectra of Gly to LA using Ru-4 at 298 K in D<sub>2</sub>O.

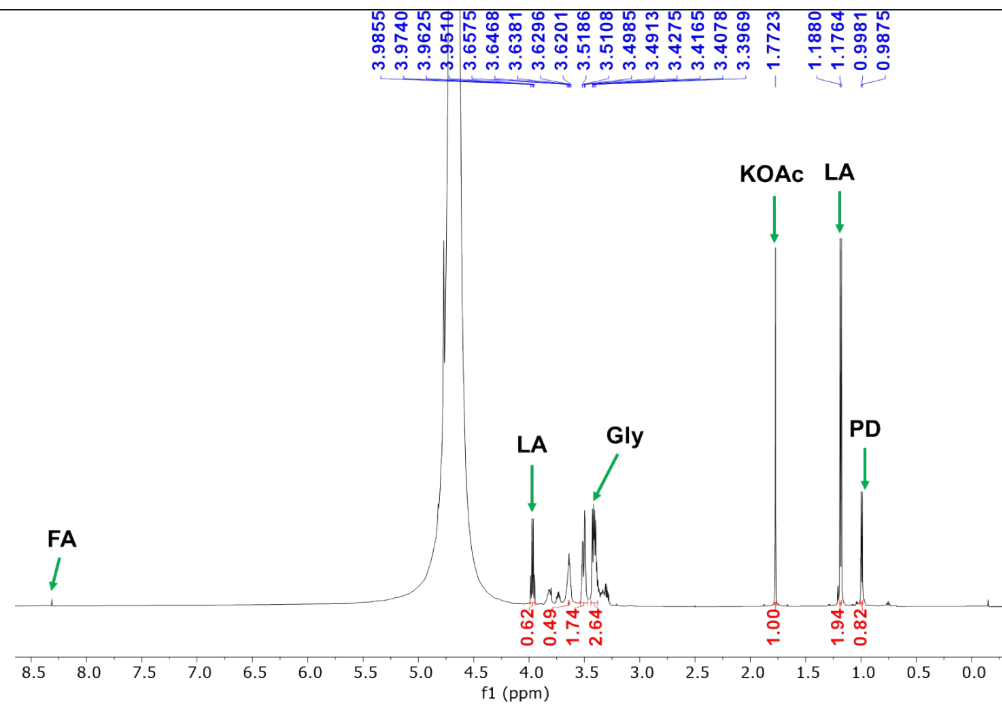


Fig. S96  $^1\text{H}$  NMR spectra of Gly to LA using Ru-5 at 298 K in D<sub>2</sub>O.

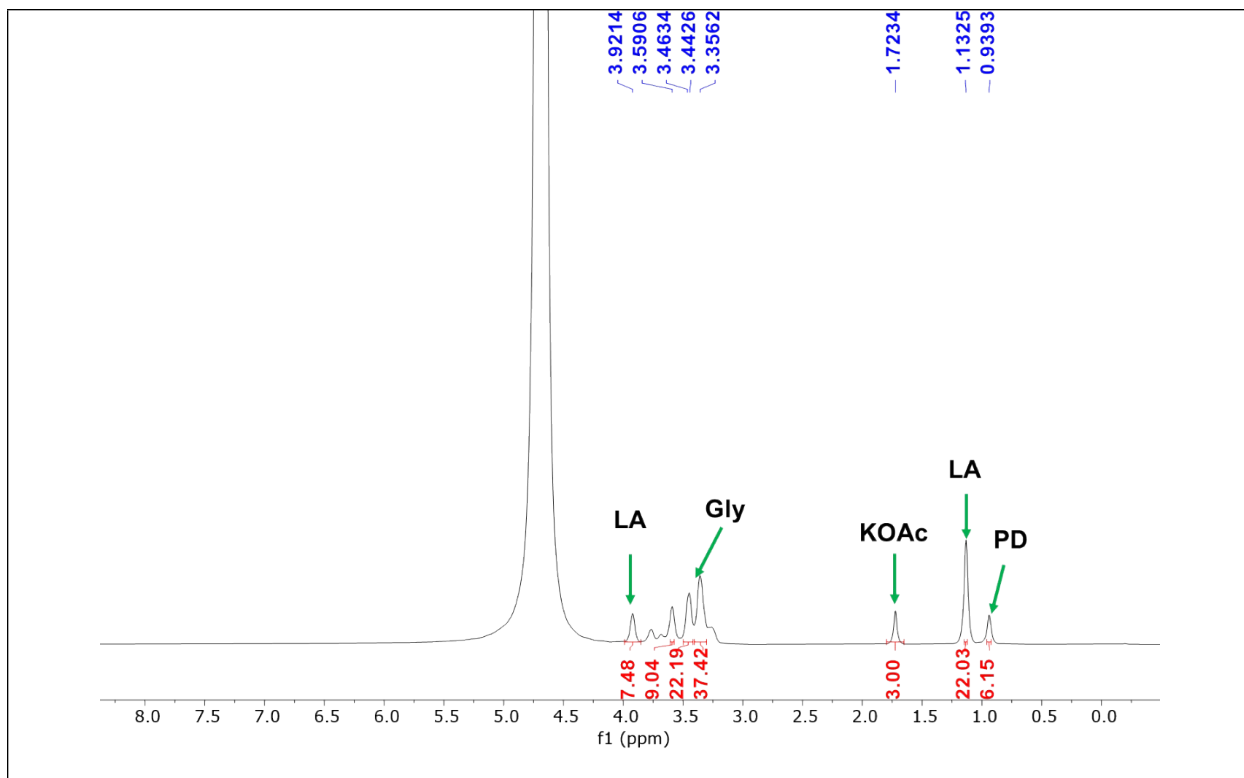
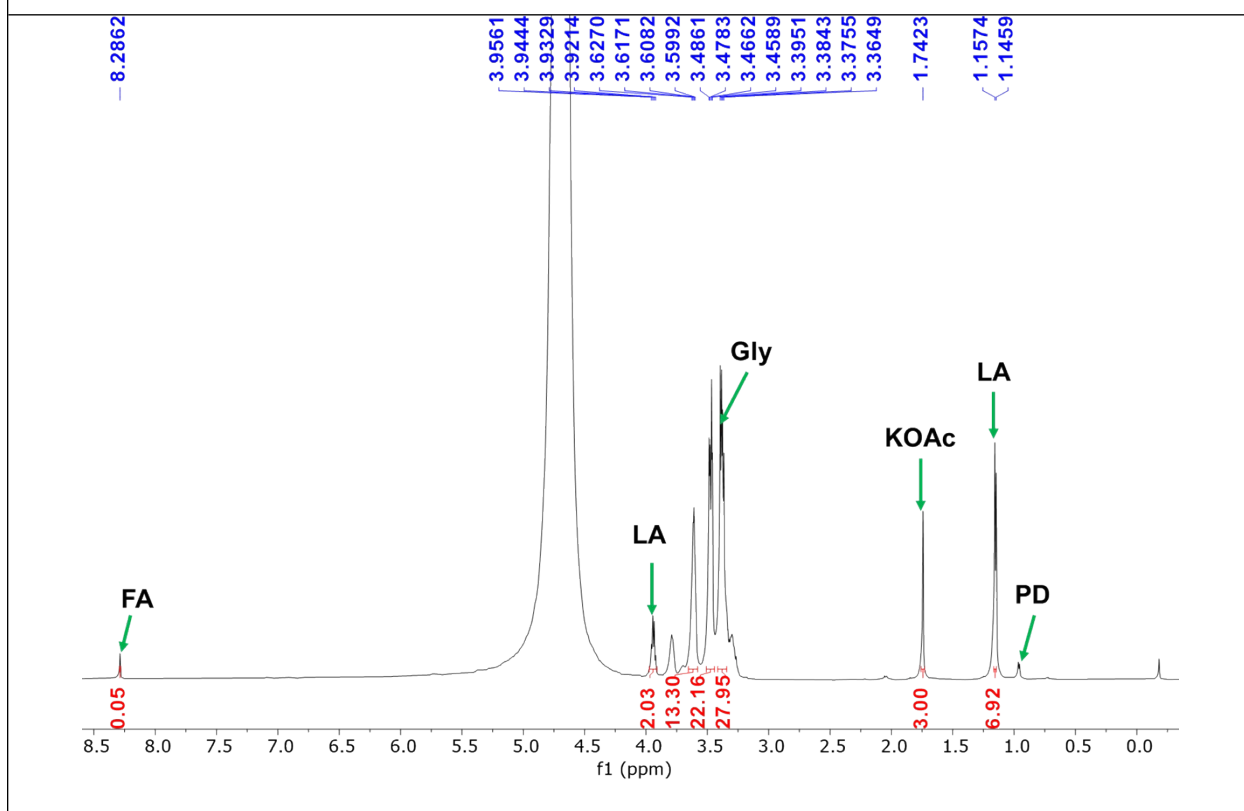
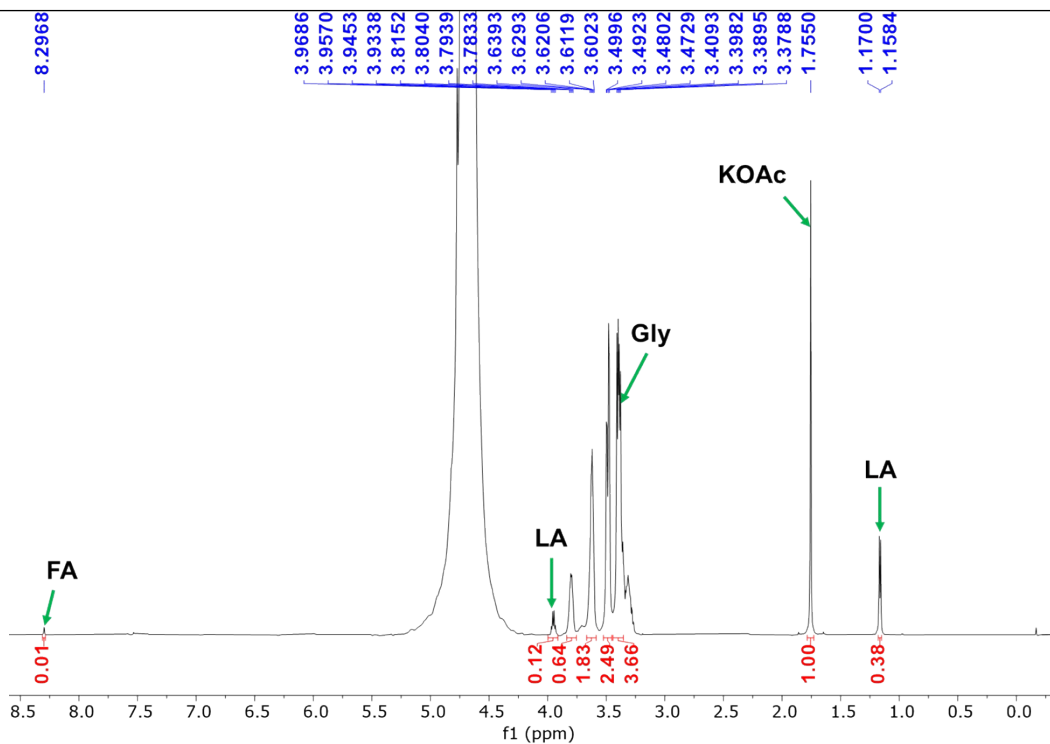


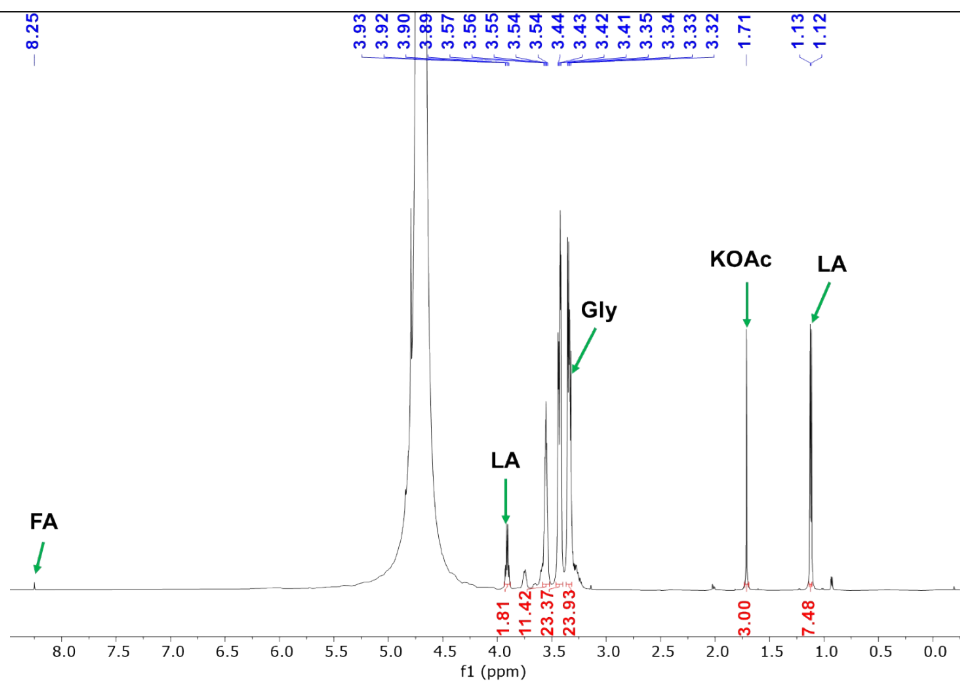
Fig. S97  $^1\text{H}$  NMR spectra of Gly to LA using Ru-6 at 298 K in  $\text{D}_2\text{O}$ .



**Fig. S98**  $^1\text{H}$  NMR spectra of **Gly** to **LA** using **Ru-7** at 298 K in  $\text{D}_2\text{O}$ .



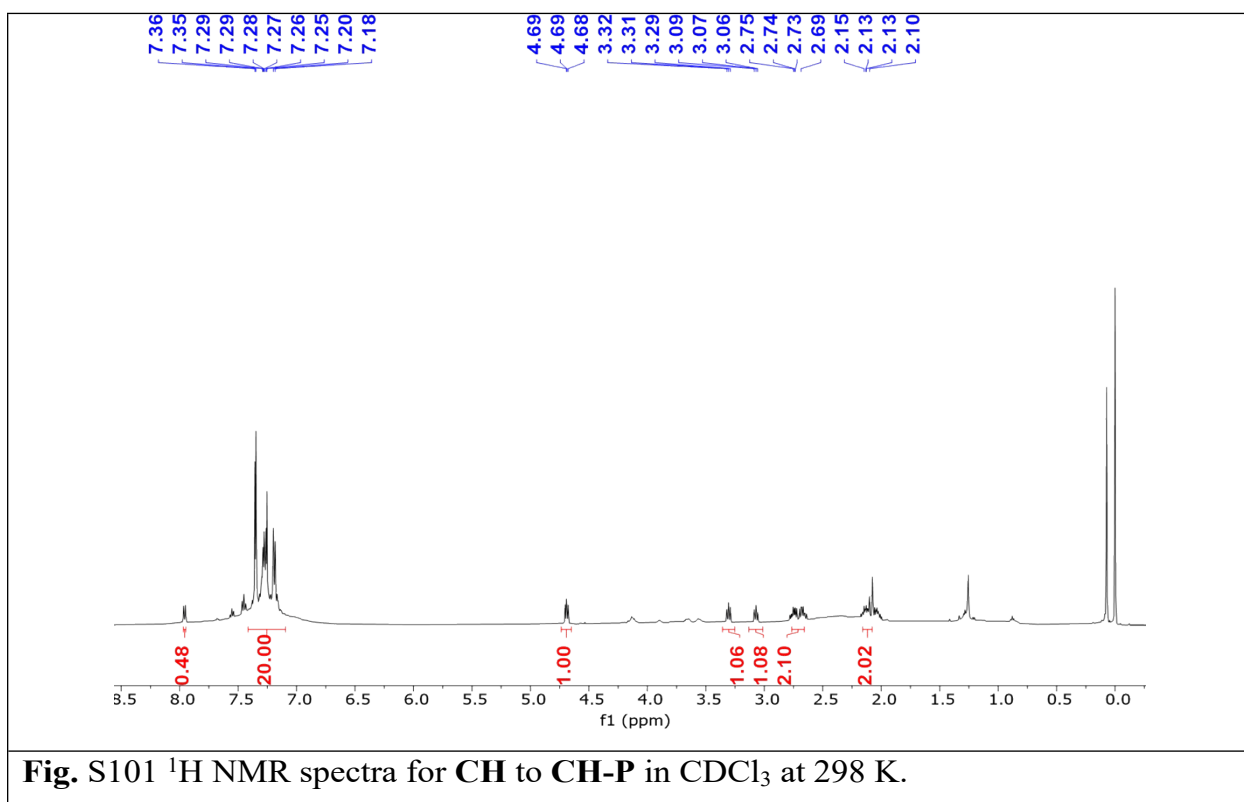
**Fig. S99**  $^1\text{H}$  NMR spectra of **Gly** to **LA** using **Ru-8** at 298 K in  $\text{D}_2\text{O}$ .

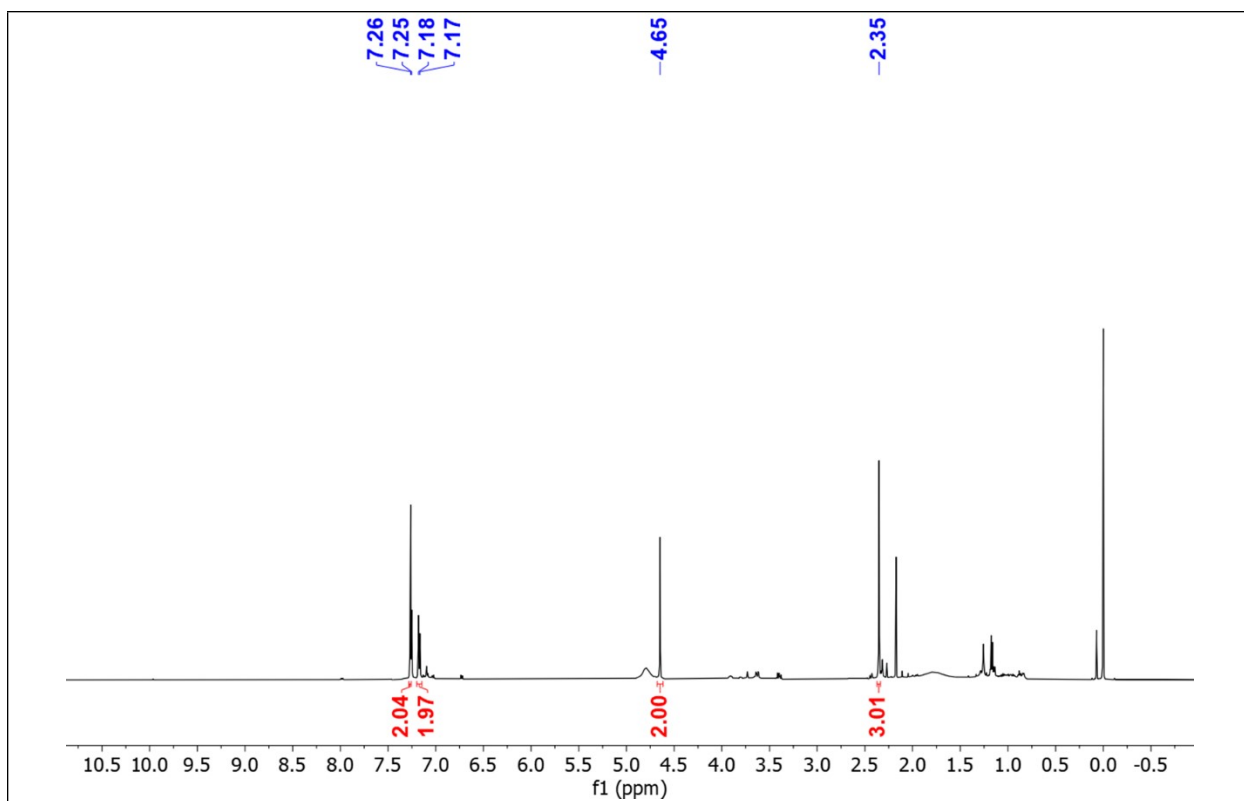


**Fig. S100**  $^1\text{H}$  NMR spectra of **Gly** to **LA** using **Ru-9** at 298 K in  $\text{D}_2\text{O}$ .

### 3.9 Utilization of in-situ generated H<sub>2</sub>

For this, glycerol (7 mmol; 0.510 mL), water (0.5 mL), NaOH (7 mmol; 0.280 g), **Ru-1** (0.05 mol%, 2.5 mg), and unsaturated substrate (chalcone and aldehyde) were placed in a 20 mL glass tube and heated at 160 °C for 24 h. After the completion of reaction, add 5 mL water to the reaction mixture and the corresponding saturated product was extracted using ethyl acetate. The solvent was evaporated and conversion was determined through <sup>1</sup>H NMR spectroscopy in CDCl<sub>3</sub>.

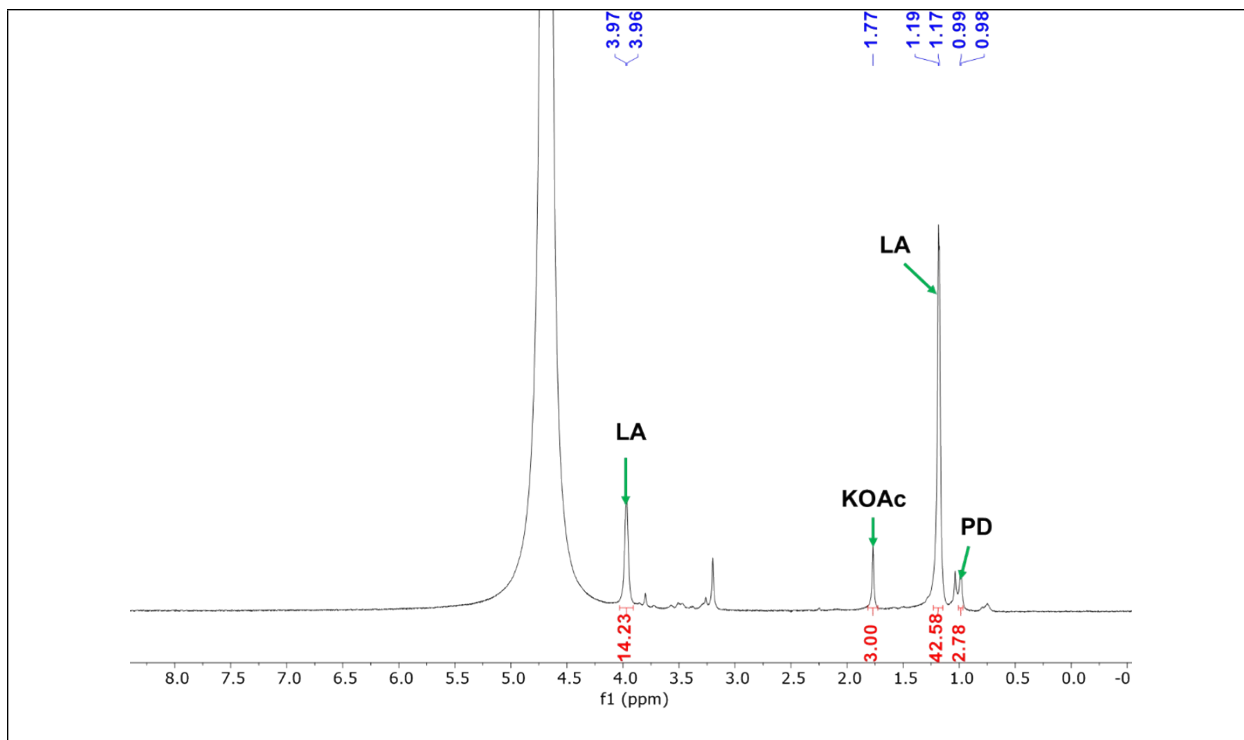




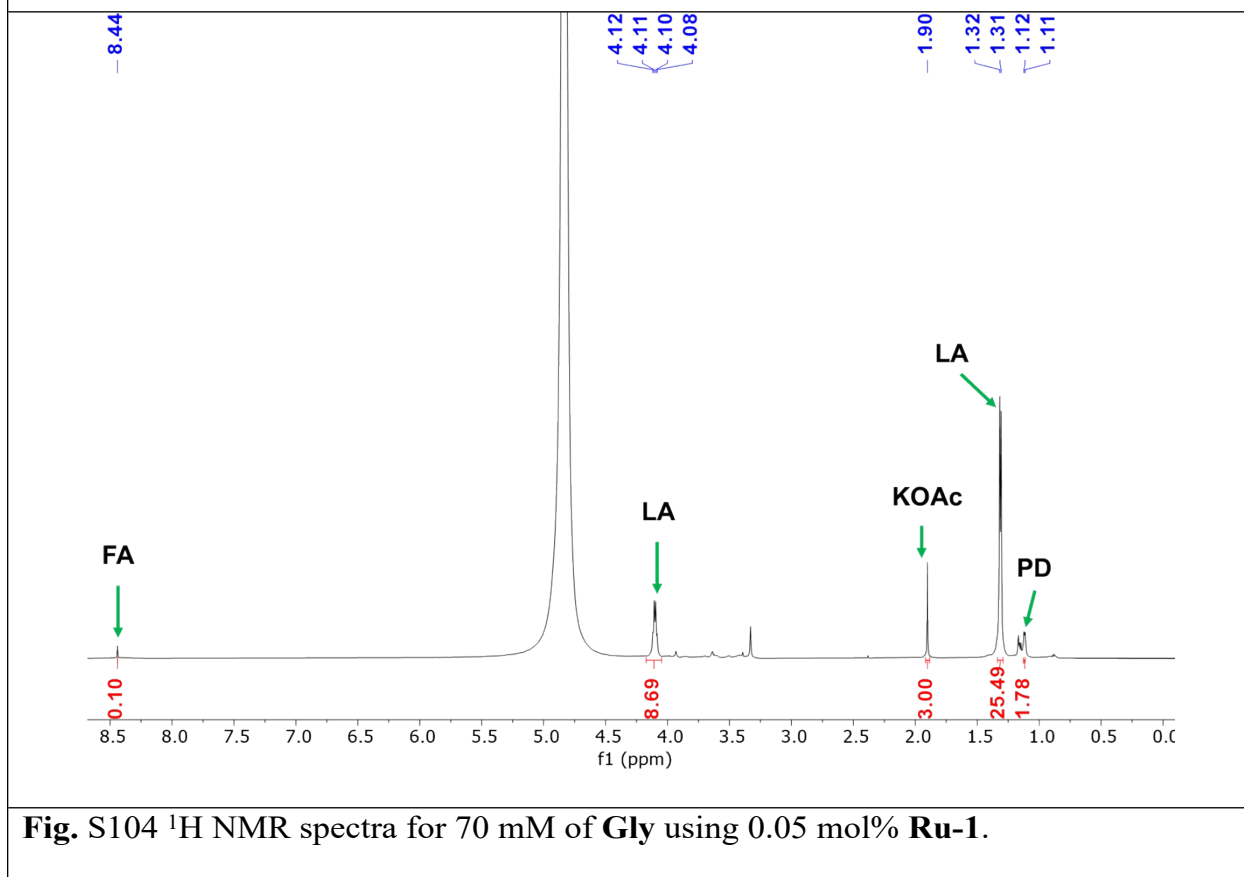
**Fig. S102**  $^1\text{H}$  NMR spectra for **4Meald** to **4Mealc** in  $\text{CDCl}_3$  at 298 K.

#### 4. Scalability

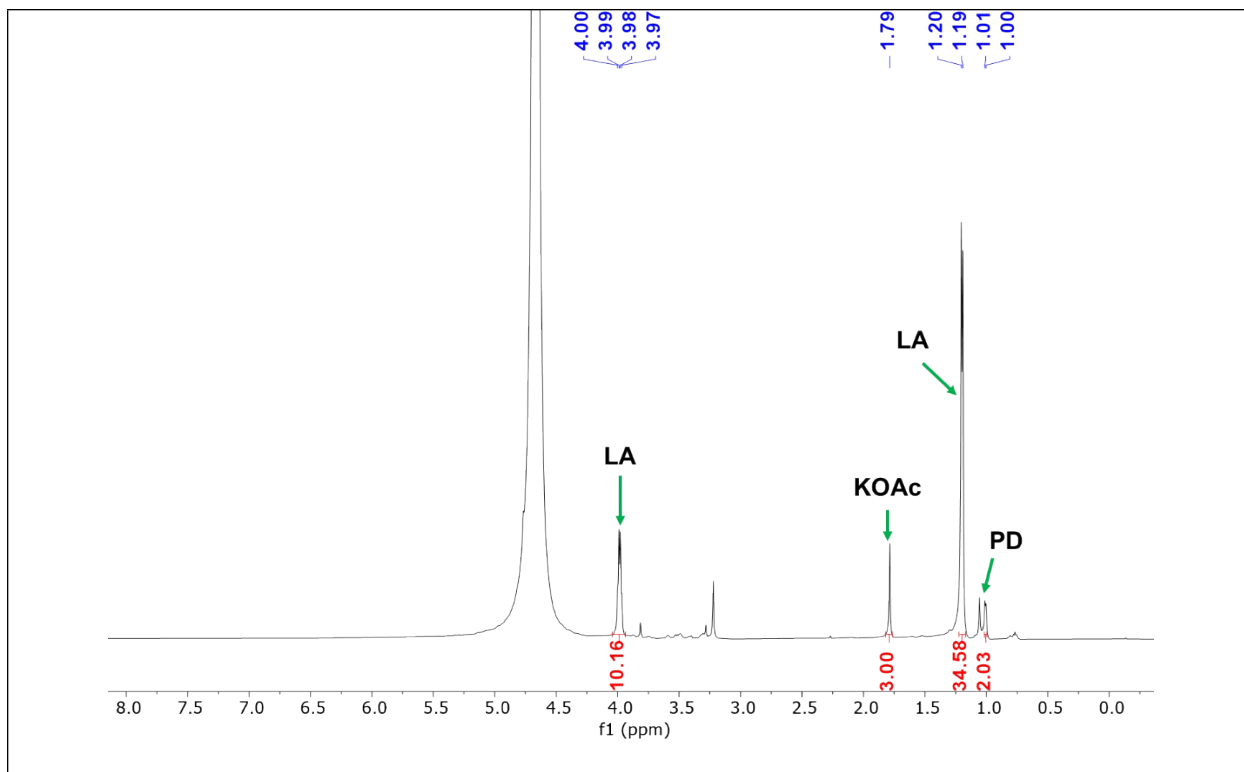
For the scalability experiments, the variable concentrations (35/70/140/210/280 mM) of glycerol were mixed with **Ru-1** (0.02/0.05 mol%) catalyst, NaOH base (1 eqv) in water in a high-pressure reactor. The mixture was stirred at 160°C for the required reaction time. After completion, water was added to the reaction mixture. The conversion of glycerol and the selectivity toward lactic acid (LA) were determined by  $^1\text{H}$  NMR spectroscopy in  $\text{D}_2\text{O}$  solvent, using KOAc as an external standard.



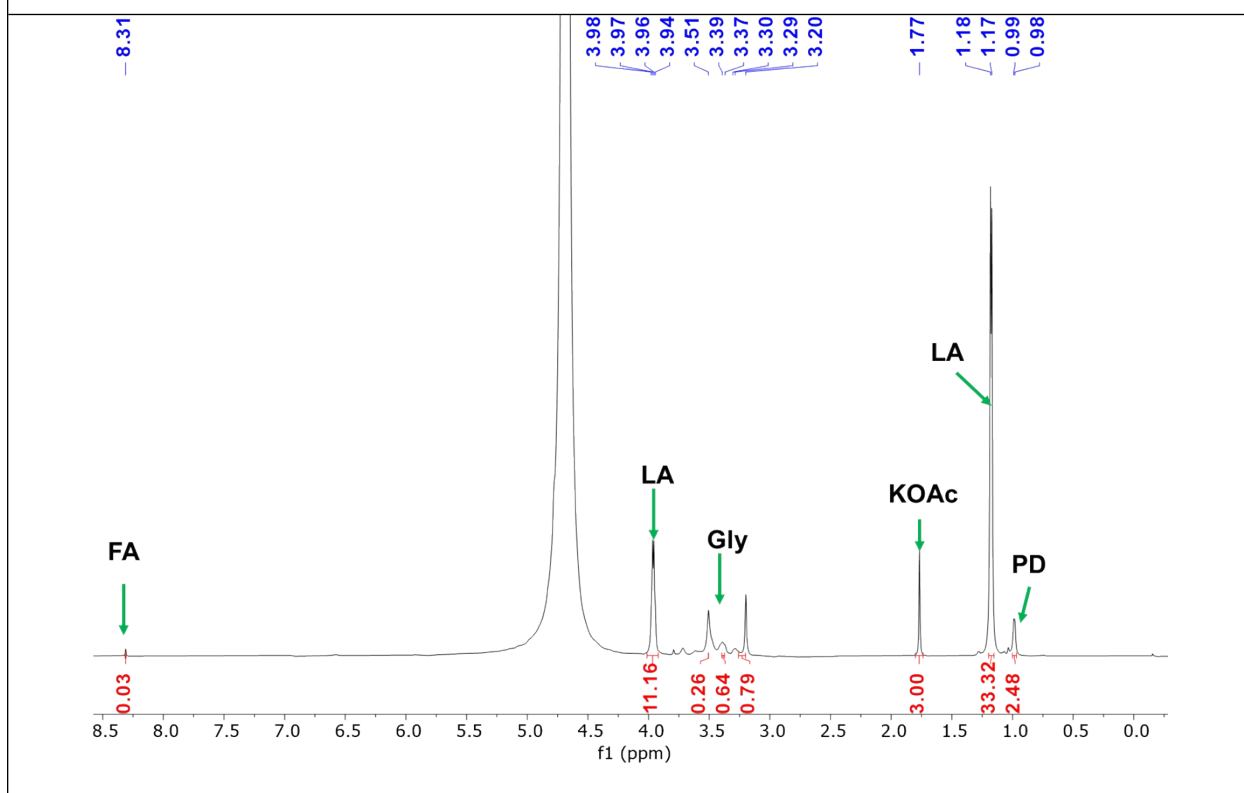
**Fig. S103**  $^1\text{H}$  NMR spectra for 35 mM of **Gly** using 0.05 mol% **Ru-1**.



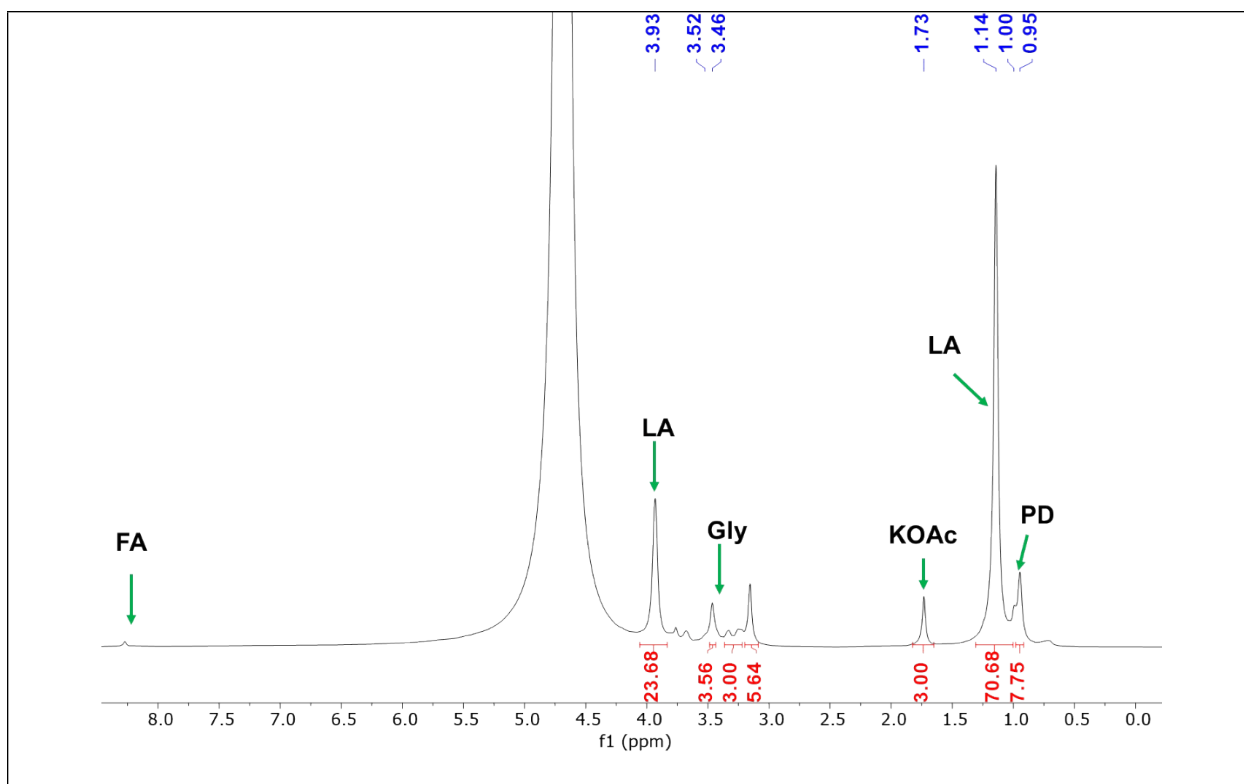
**Fig. S104**  $^1\text{H}$  NMR spectra for 70 mM of **Gly** using 0.05 mol% **Ru-1**.



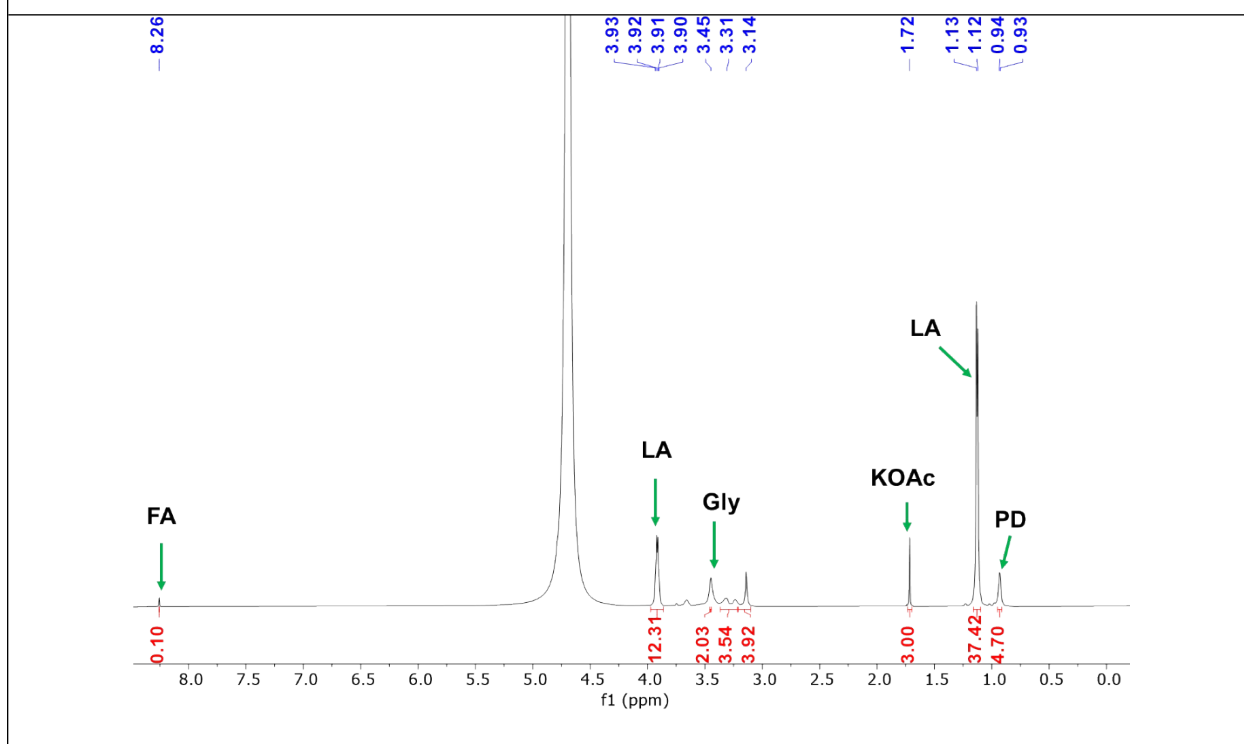
**Fig. S105**  $^1\text{H}$  NMR spectra for 140 mM of **Gly** using 0.05 mol% **Ru-1**.



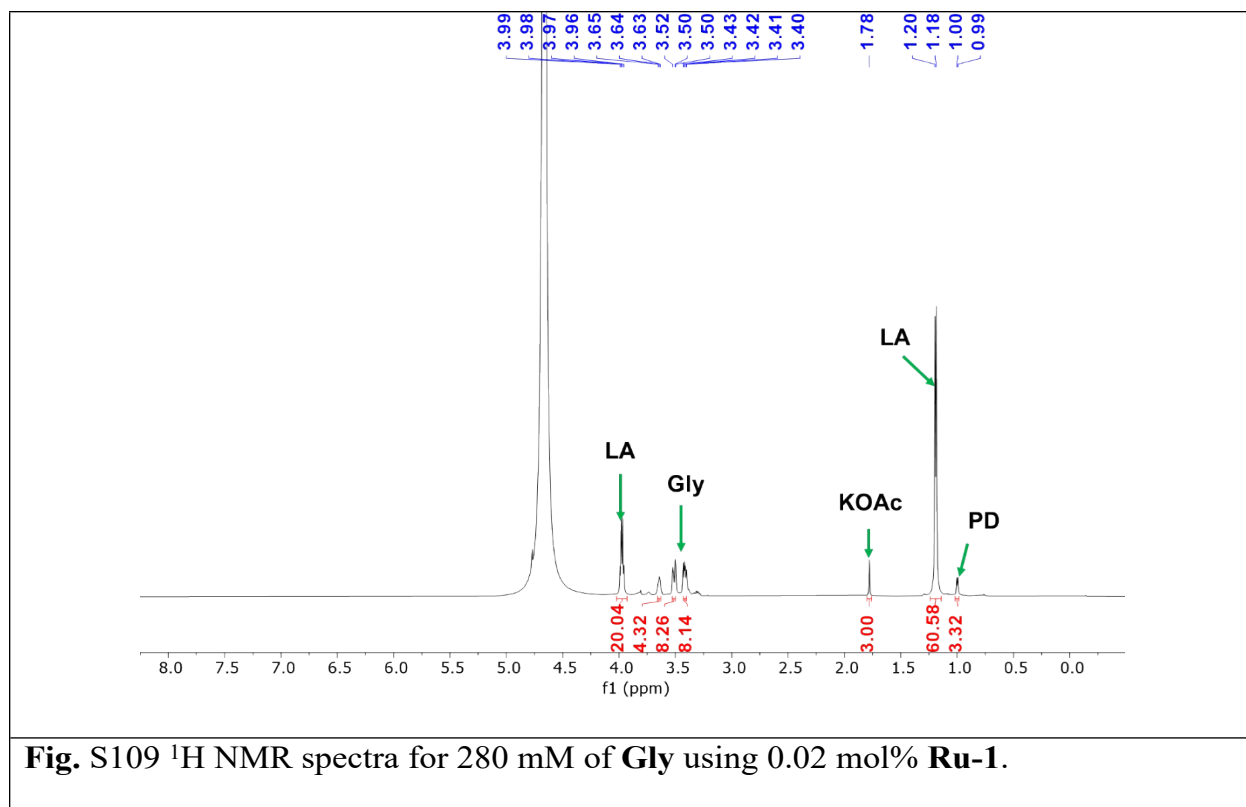
**Fig. S106**  $^1\text{H}$  NMR spectra for 70 mM of **Gly** using 0.02 mol% **Ru-1**.



**Fig. S107**  $^1\text{H}$  NMR spectra for 140 mM of **Gly** using 0.02 mol% **Ru-1**.



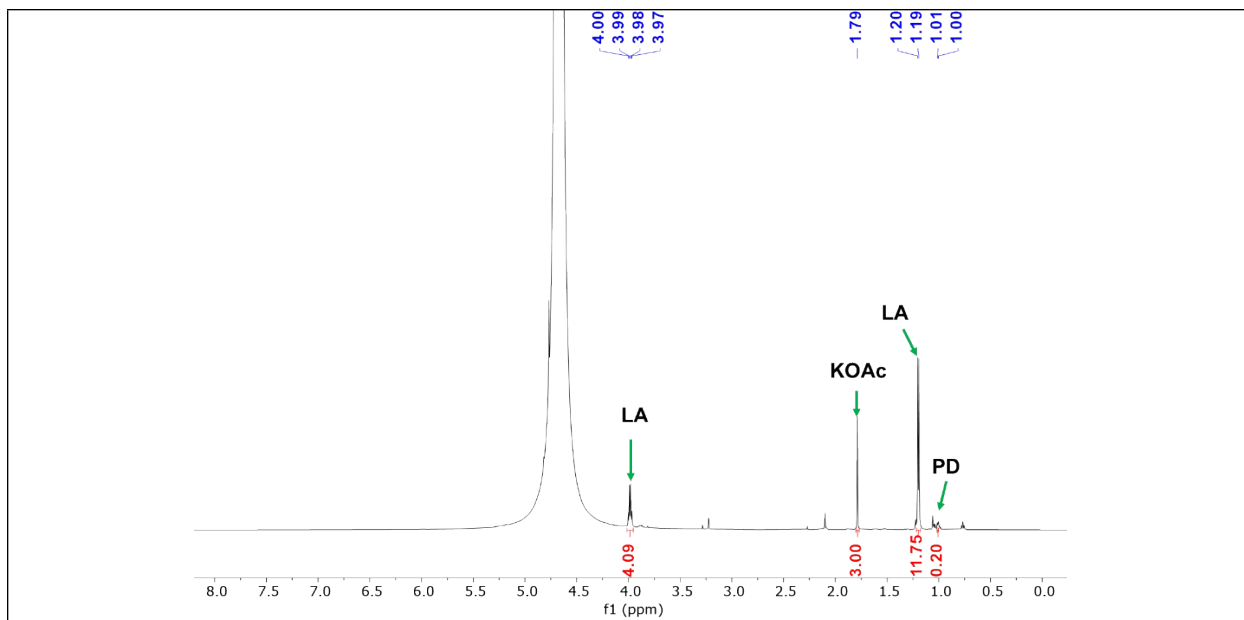
**Fig. S108**  $^1\text{H}$  NMR spectra for 210 mM of **Gly** using 0.02 mol% **Ru-1**.



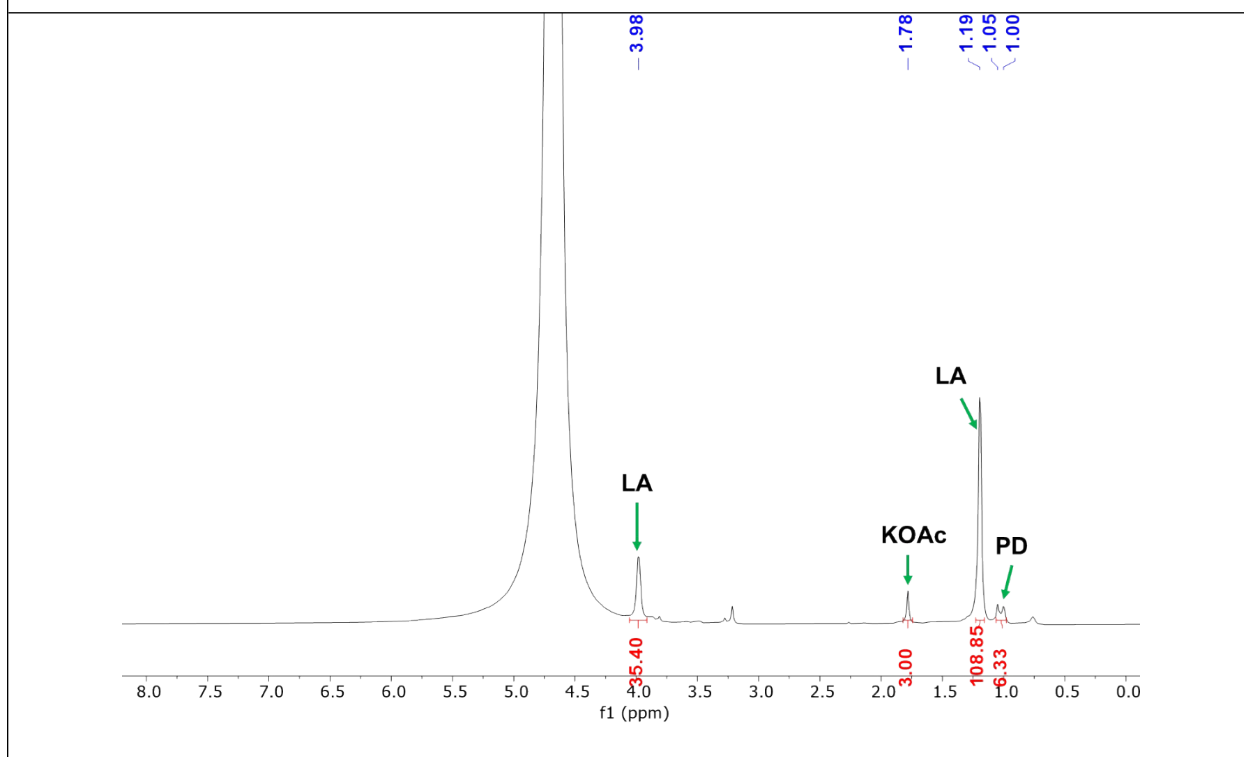
## 5. Reusability

### General Procedure

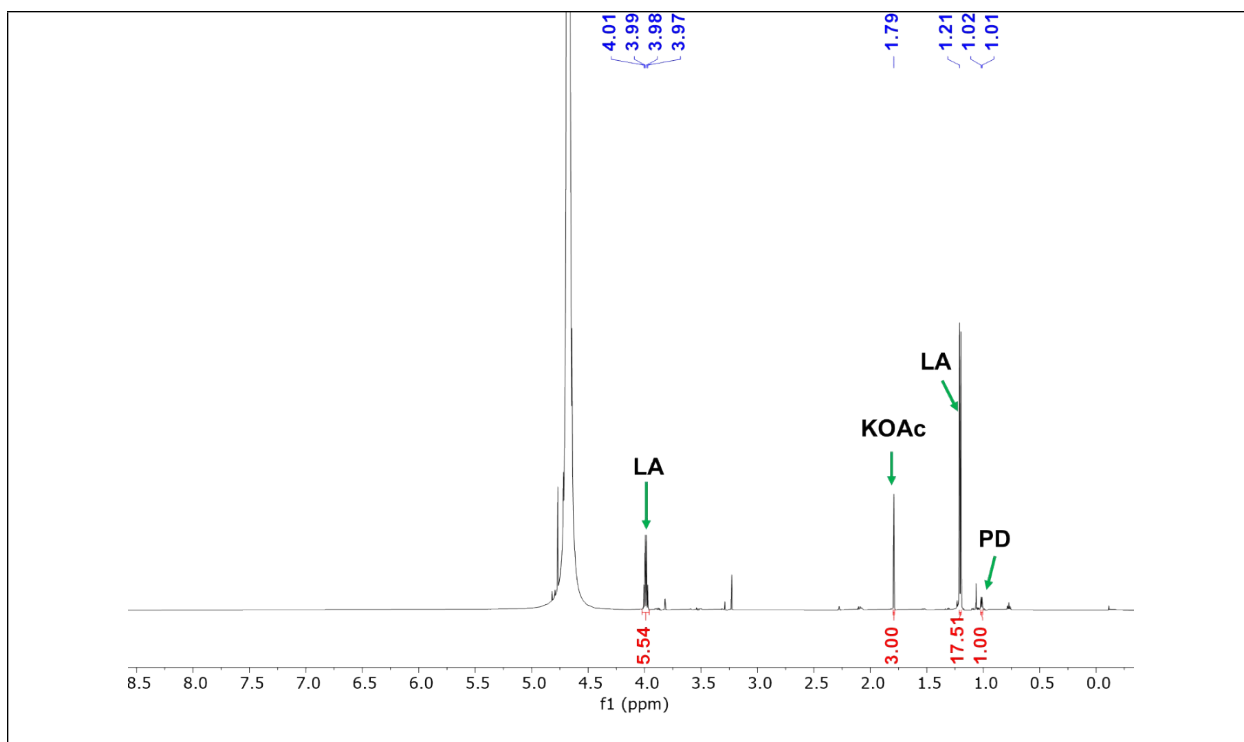
For the reusability studies, the catalytic dehydrogenation of glycerol (35 mmol, 2.55 mL) was performed with **Ru-1** (20 mg) and NaOH (1 equiv.) in 2.45 mL of water at 160 °C for 24 h in a high-pressure reactor. After the first reaction cycle, a 100  $\mu\text{L}$  aliquot was withdrawn and analyzed by  $^1\text{H}$  NMR spectroscopy to determine conversion. The reactor was then recharged with fresh glycerol (35 mmol, 2.55 mL), NaOH (1 equiv.), and 2.45 mL of water, without adding additional **Ru-1** catalyst. This procedure was repeated for each subsequent cycle using the same catalyst batch. **Ru-1** was successfully reused for 10 consecutive cycles, consistently affording good to excellent conversions in all runs. Conversions for each cycle were quantified by  $^1\text{H}$  NMR spectroscopy, confirming the robustness and sustained activity of the catalyst under the conditions. These findings highlight the reusability of **Ru-1** and its strong potential for practical applications in homogeneous dehydrogenation processes.



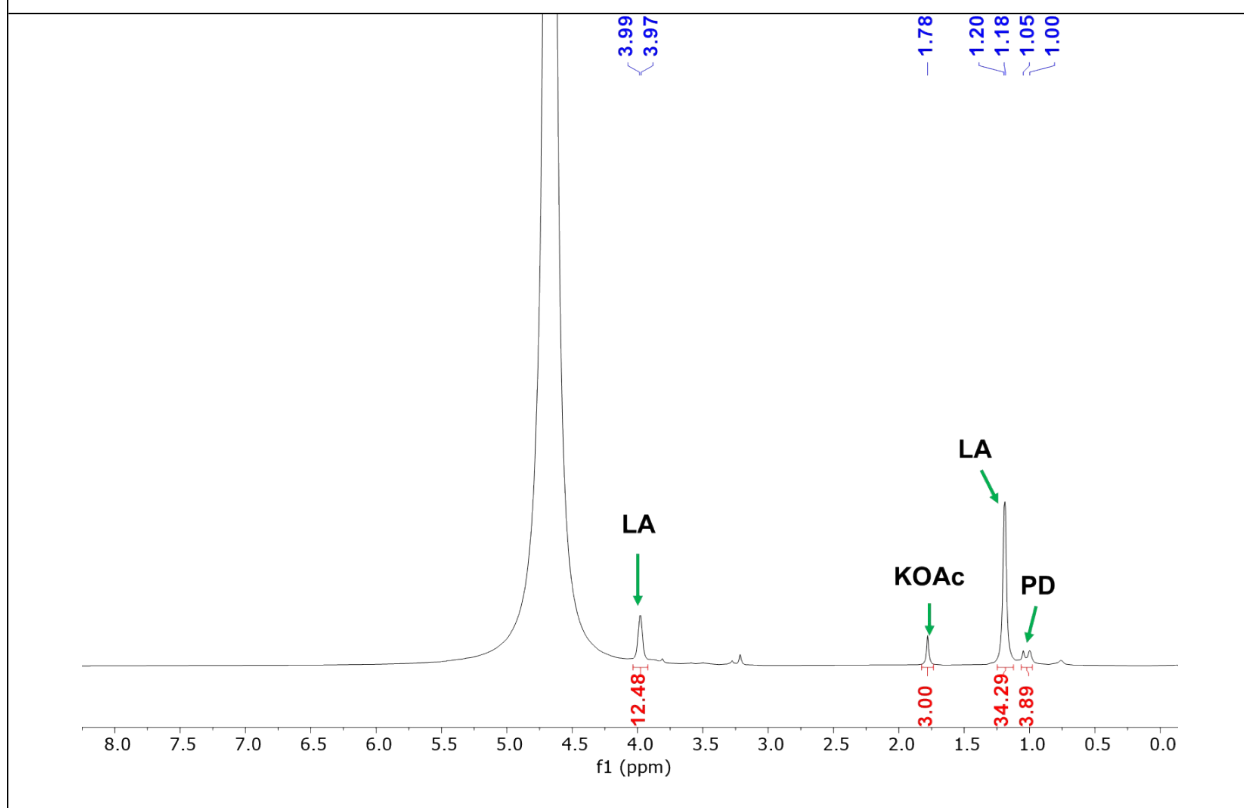
**Fig. S110**  $^1\text{H}$  NMR spectra showing the reusability of **Ru-1** in cycle 1.



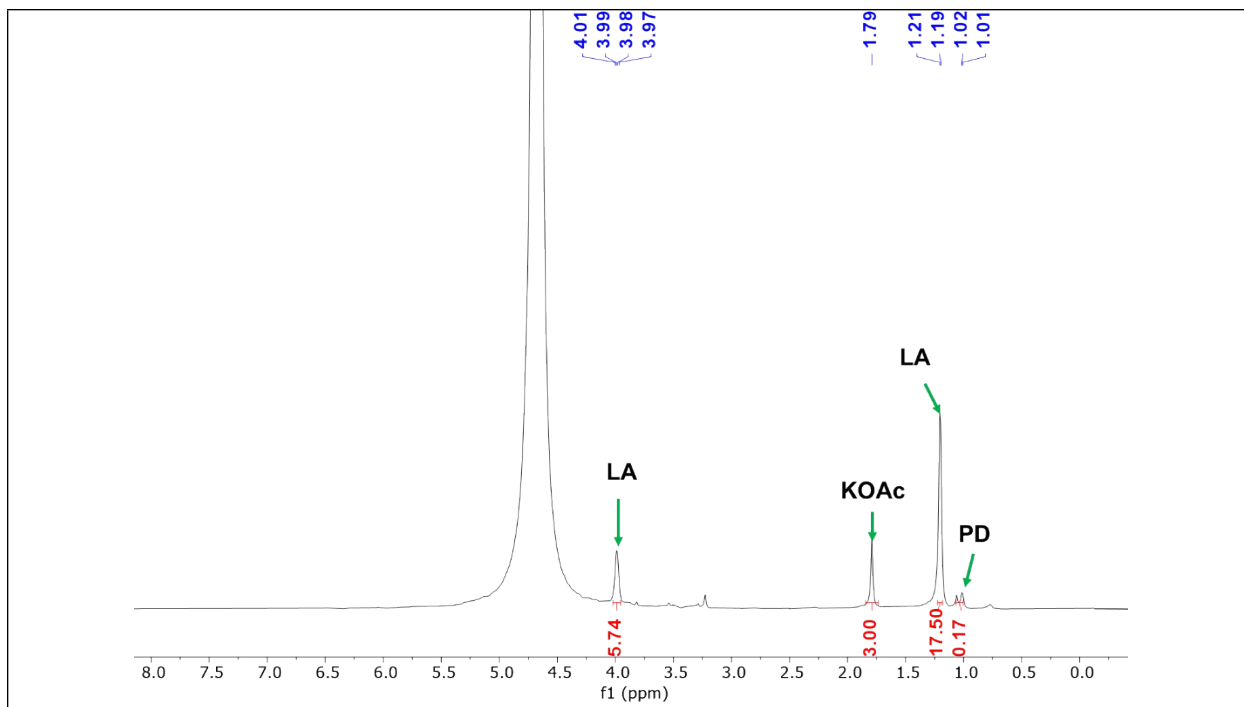
**Fig. S111**  $^1\text{H}$  NMR spectra showing the reusability of **Ru-1** in cycle 2.



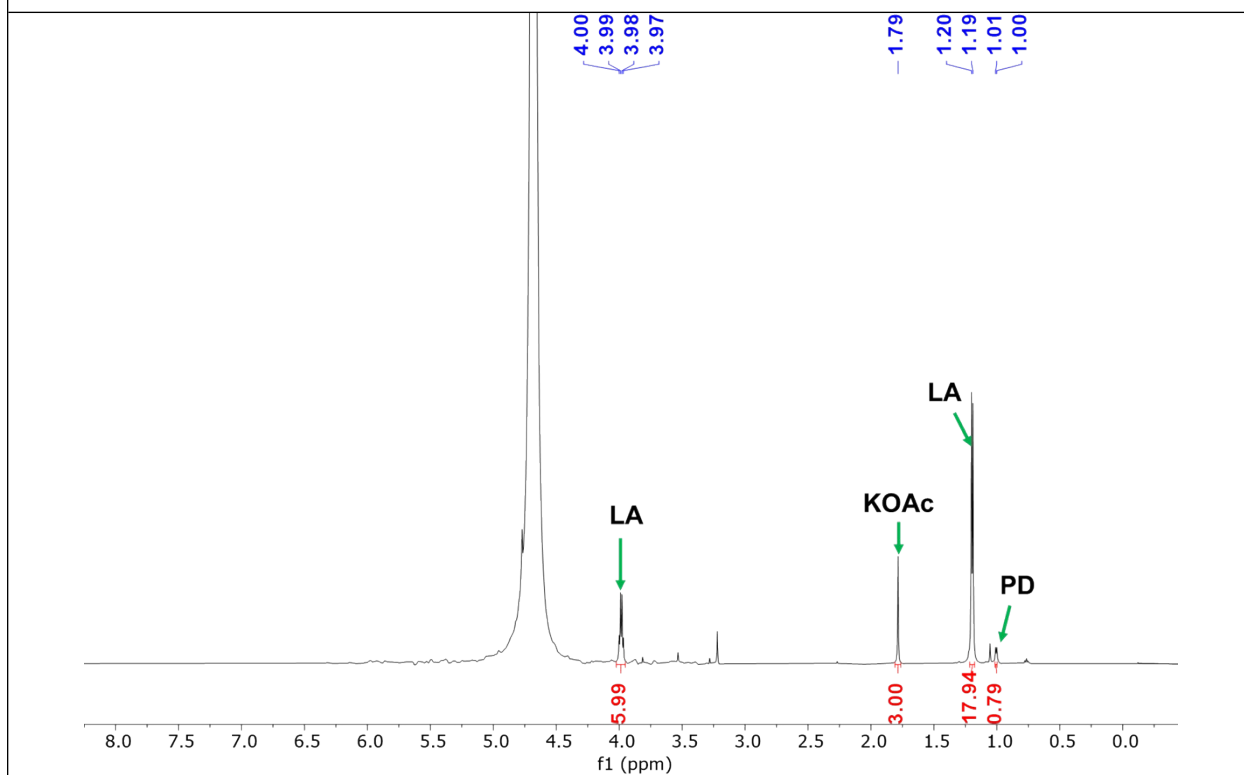
**Fig. S112**  $^1\text{H}$  NMR spectra showing the reusability of **Ru-1** in cycle 3.



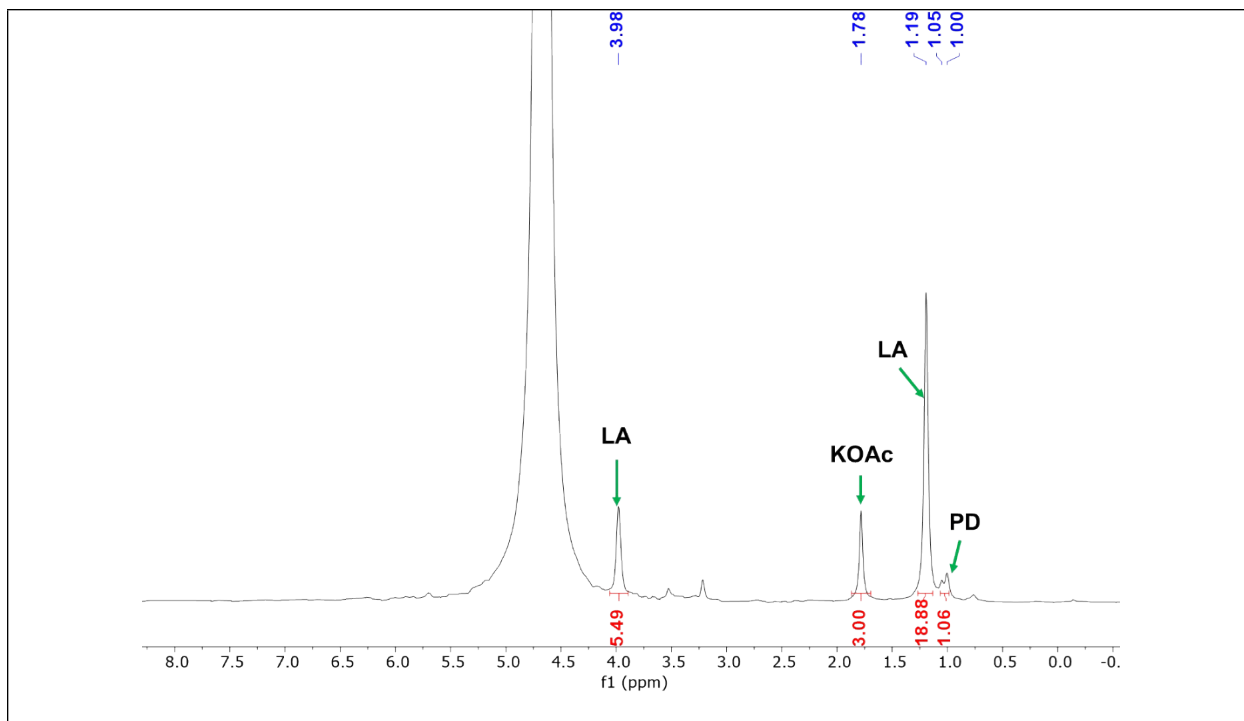
**Fig. S113**  $^1\text{H}$  NMR spectra showing the reusability of **Ru-1** in cycle 4.



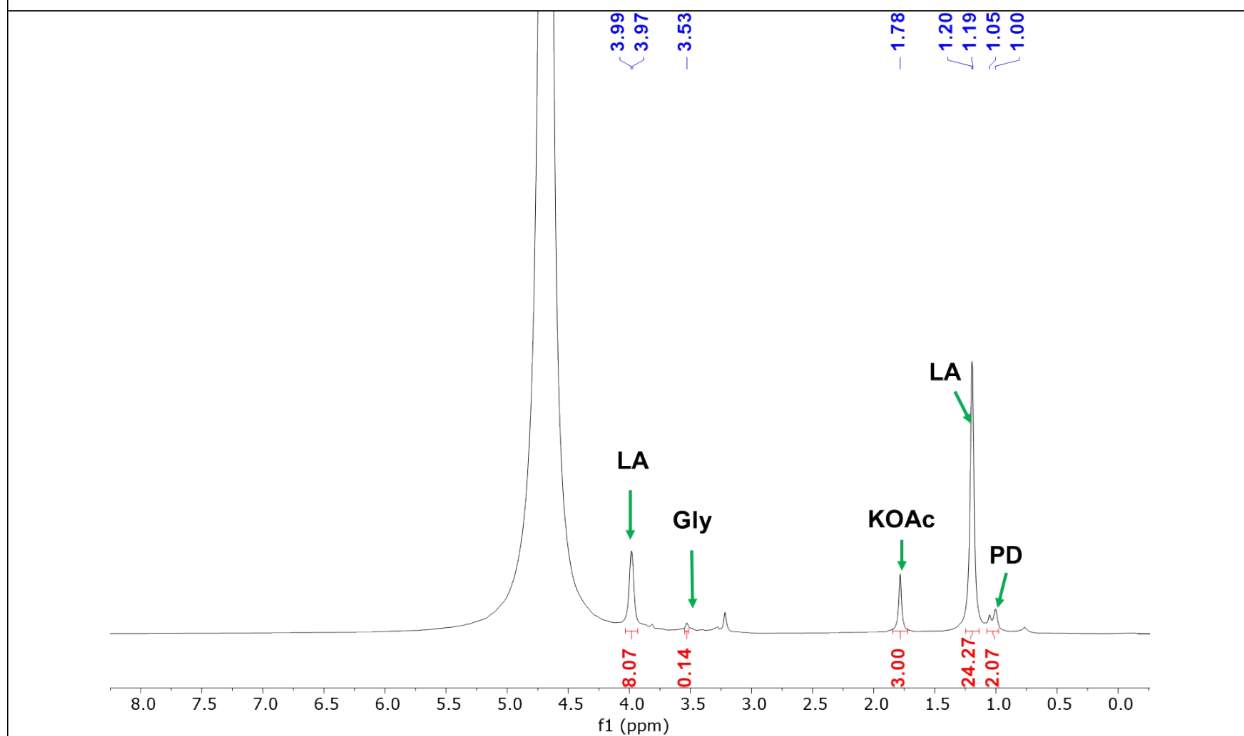
**Fig. S114**  $^1\text{H}$  NMR spectra showing the reusability of **Ru-1** in cycle 5.



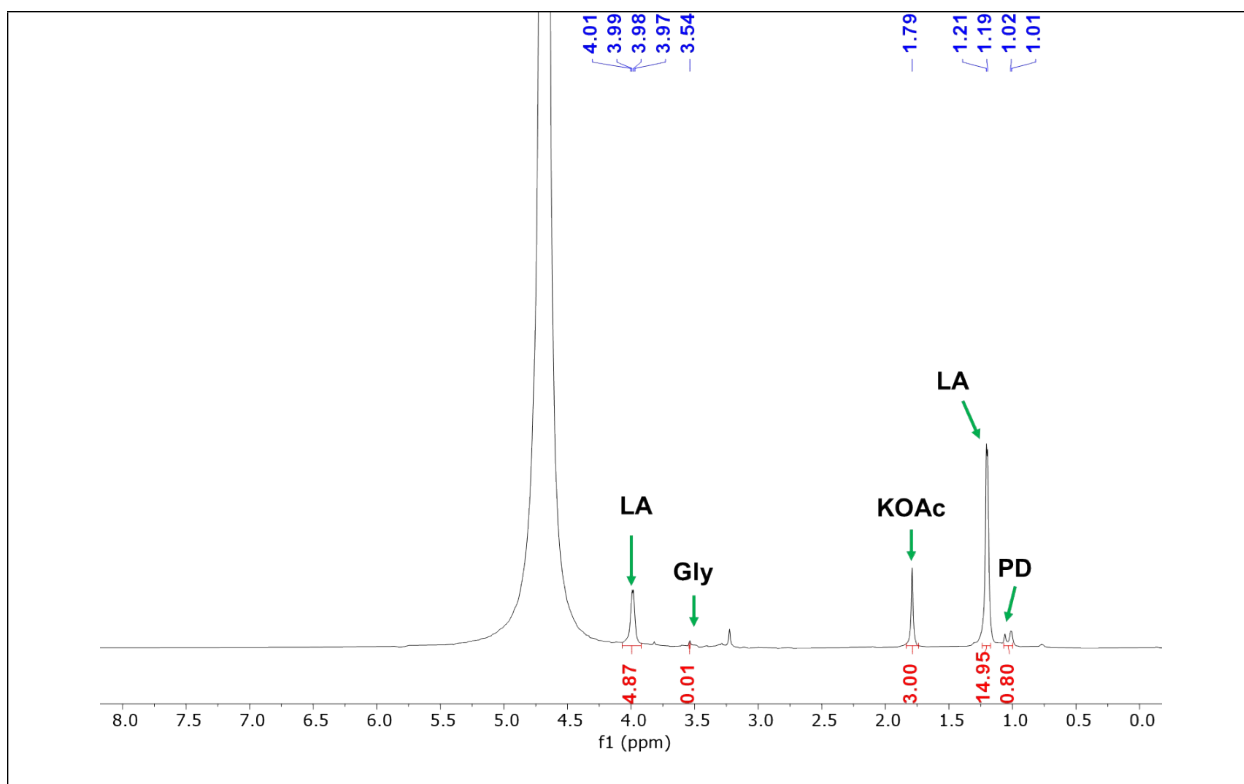
**Fig. S115**  $^1\text{H}$  NMR spectra showing the reusability of **Ru-1** in cycle 6.



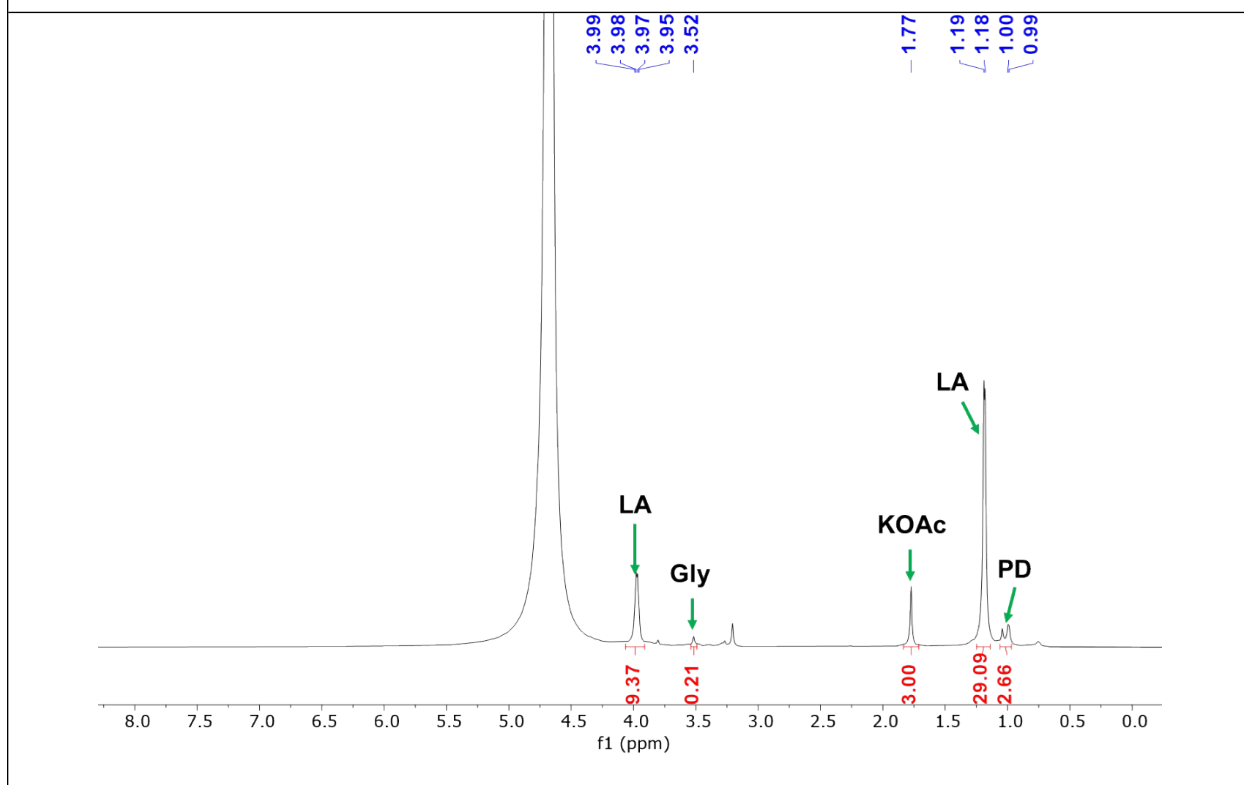
**Fig. S116**  $^1\text{H}$  NMR spectra showing the reusability of **Ru-1** in cycle 7.



**Fig. S117**  $^1\text{H}$  NMR spectra showing the reusability of **Ru-1** in cycle 8.



**Fig. S118**  $^1\text{H}$  NMR spectra showing the reusability of **Ru-1** in cycle 9.



**Fig. S119**  $^1\text{H}$  NMR spectra showing the reusability of **Ru-1** in cycle 10.

## 6. Mechanistic Study

### 6.1 Controlled experiments

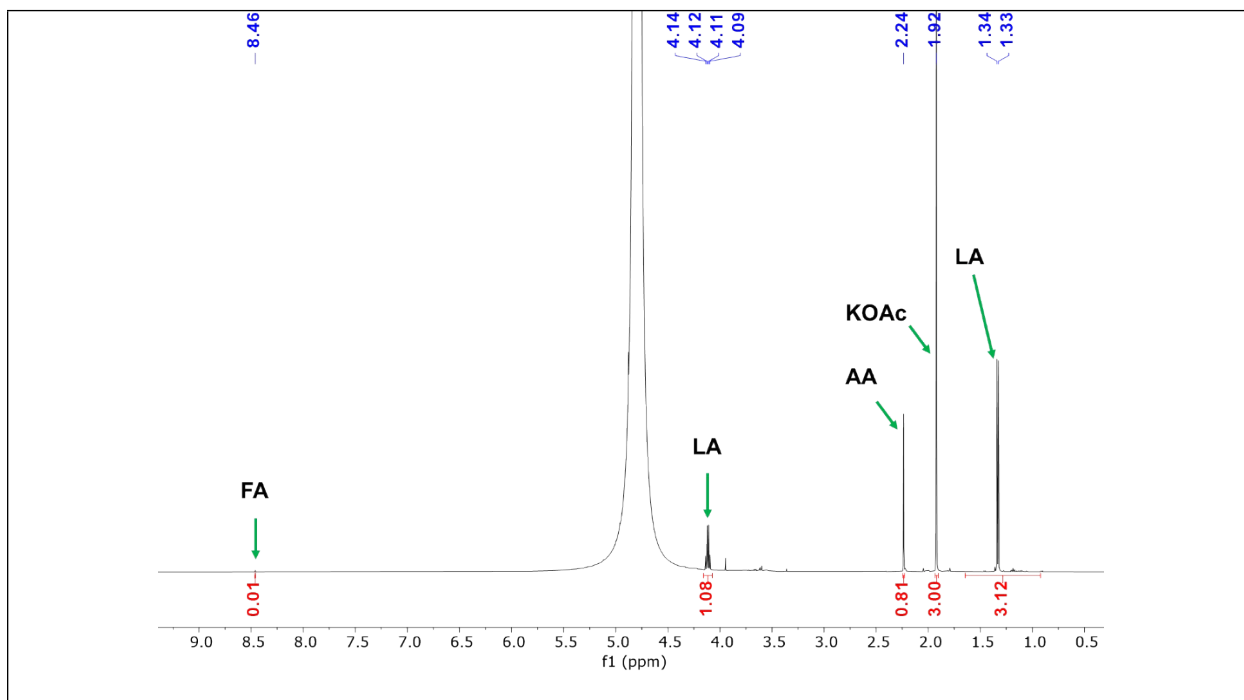


Fig. S120 <sup>1</sup>H NMR spectra for 1,2-dihydroxyacetone (DHA) to lactic acid (LA).

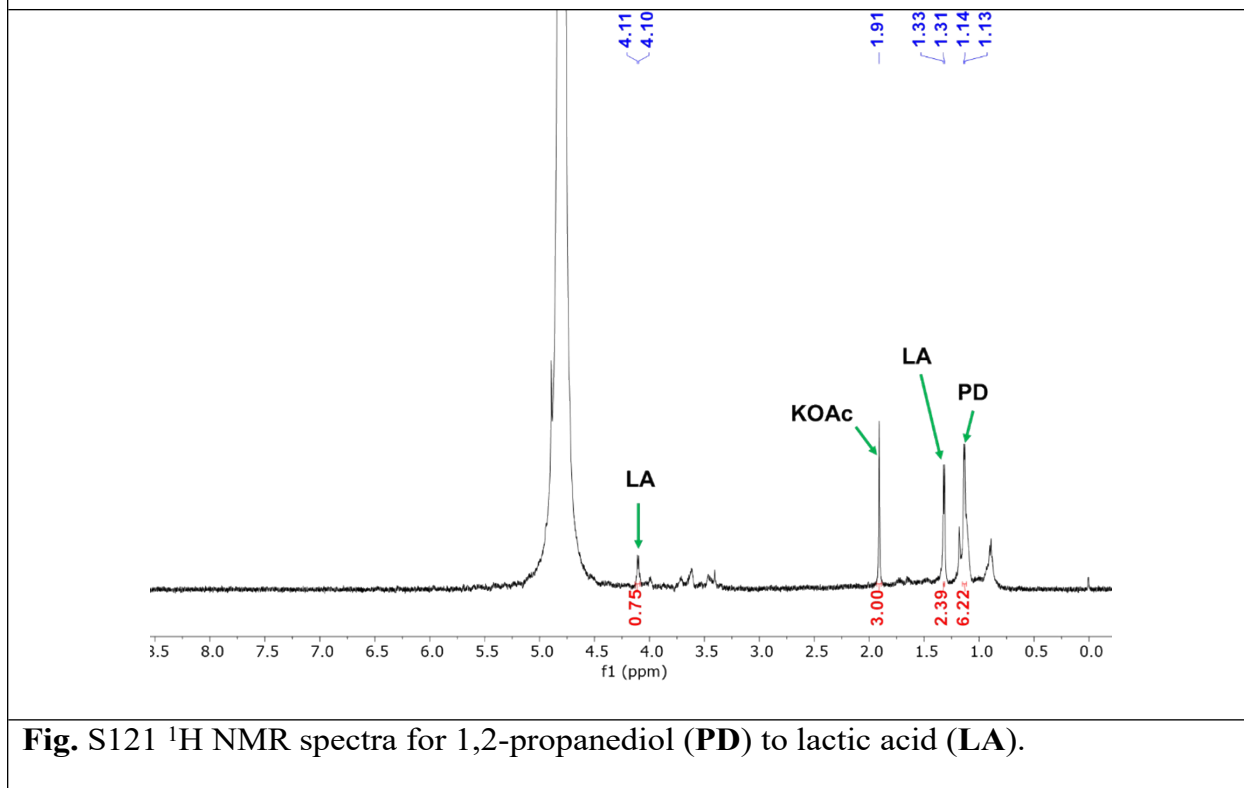
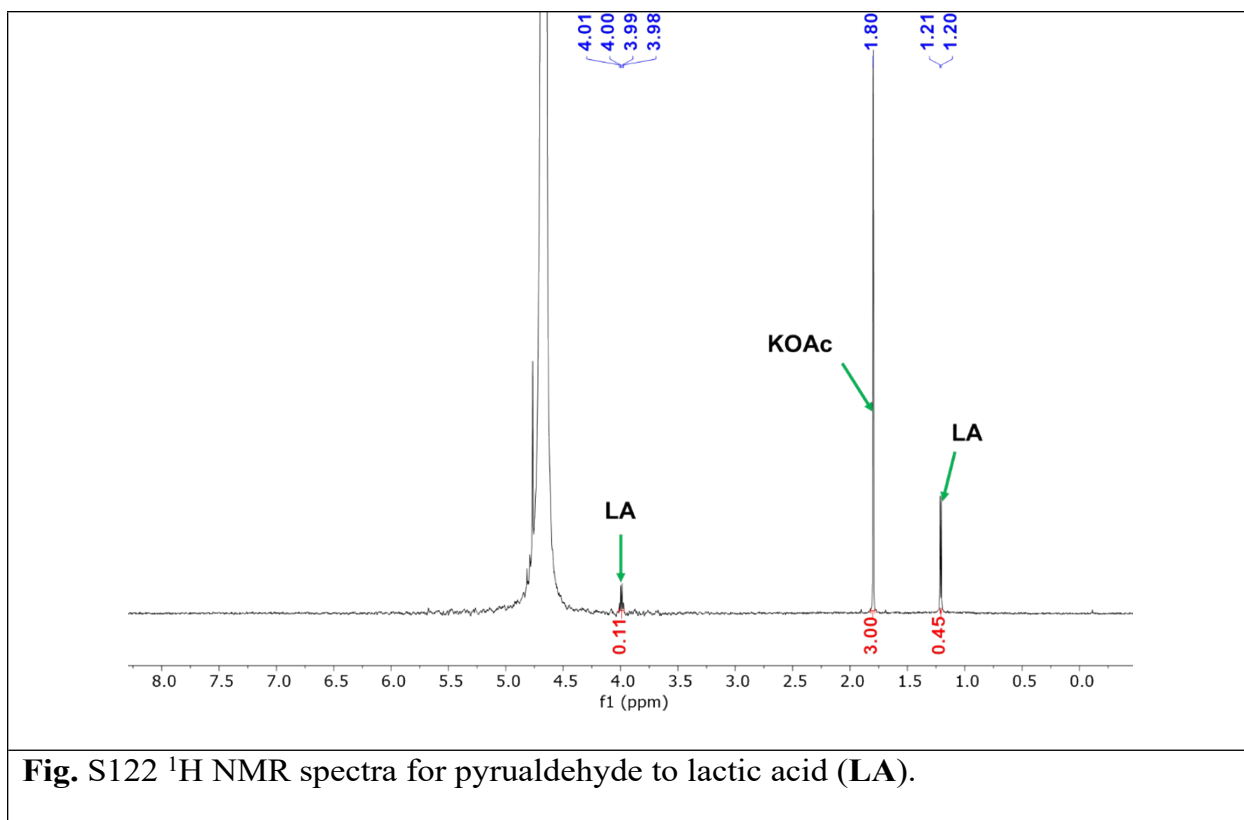


Fig. S121 <sup>1</sup>H NMR spectra for 1,2-propanediol (PD) to lactic acid (LA).



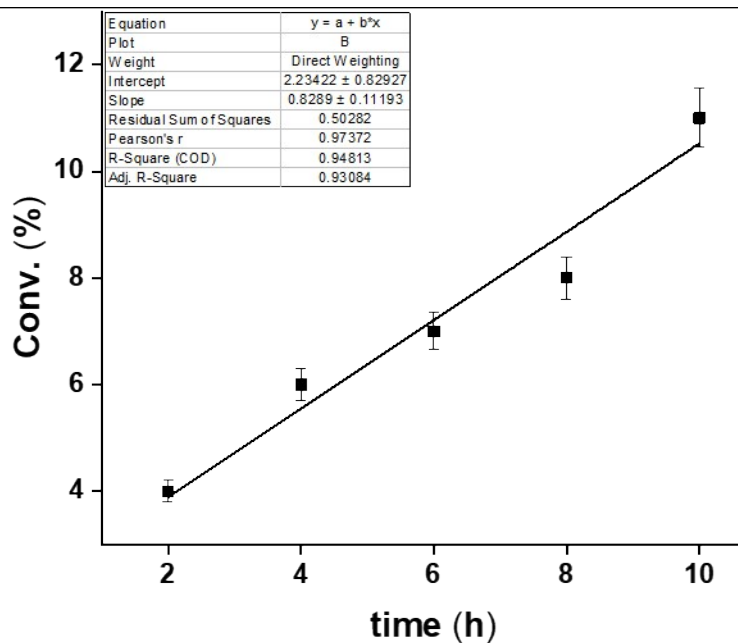
**Fig. S122**  $^1\text{H}$  NMR spectra for pyruvaldehyde to lactic acid (LA).

## 6.2 Kinetic analysis

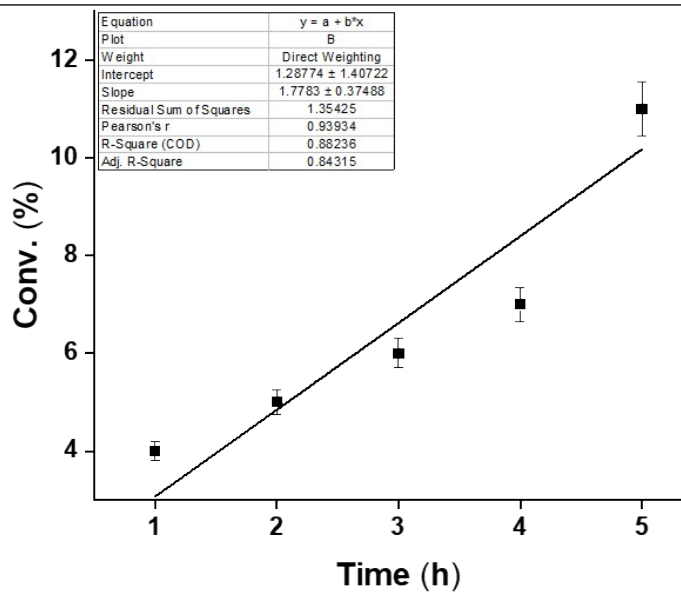
### Determination of activation parameter

For this, glycerol (7 mmol; 0.510 mL), water (0.5 mL), NaOH (7 mmol; 0.280 g), and **Ru-1** (0.05 mol%, 2.5 mg) were placed in a 20 mL glass tube and heated at temperature 413 K and take samples at variable times. The conversion of glycerol was determined through  $^1\text{H}$  NMR spectroscopy in  $\text{D}_2\text{O}$  solvent, using KOAc as an external standard. Plot the graph between conversion (%) vs time (h).

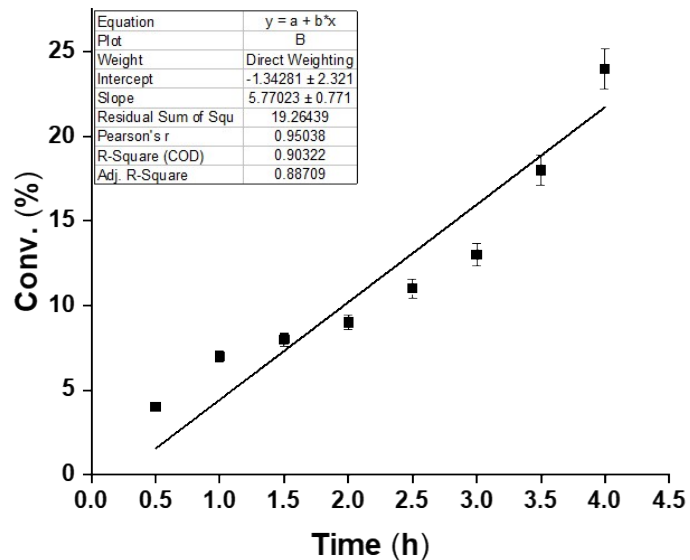
Similar procedure at variable temperatures such as 423 K, 433 K, and 443 K. Determine conversion with respect to time and plot graph between conversion (%) vs time (h) for each temperature.



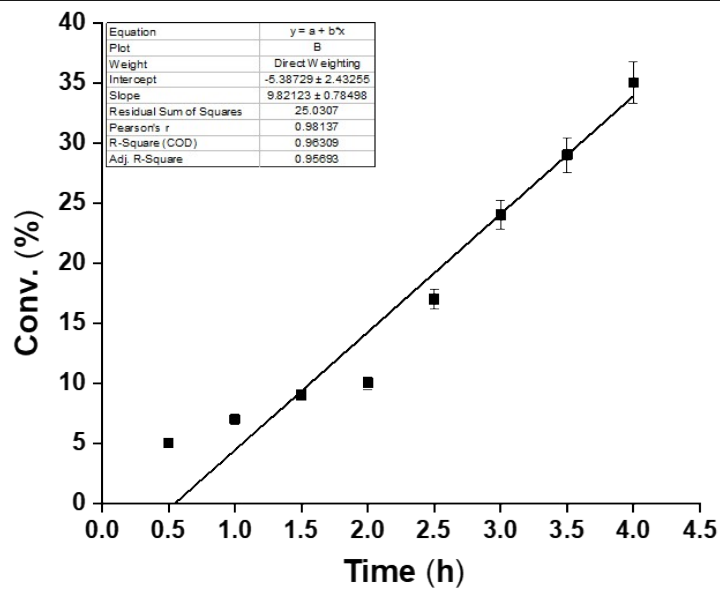
**Fig. S123** Plot of Conversion (%) vs time (h) at 413 K.



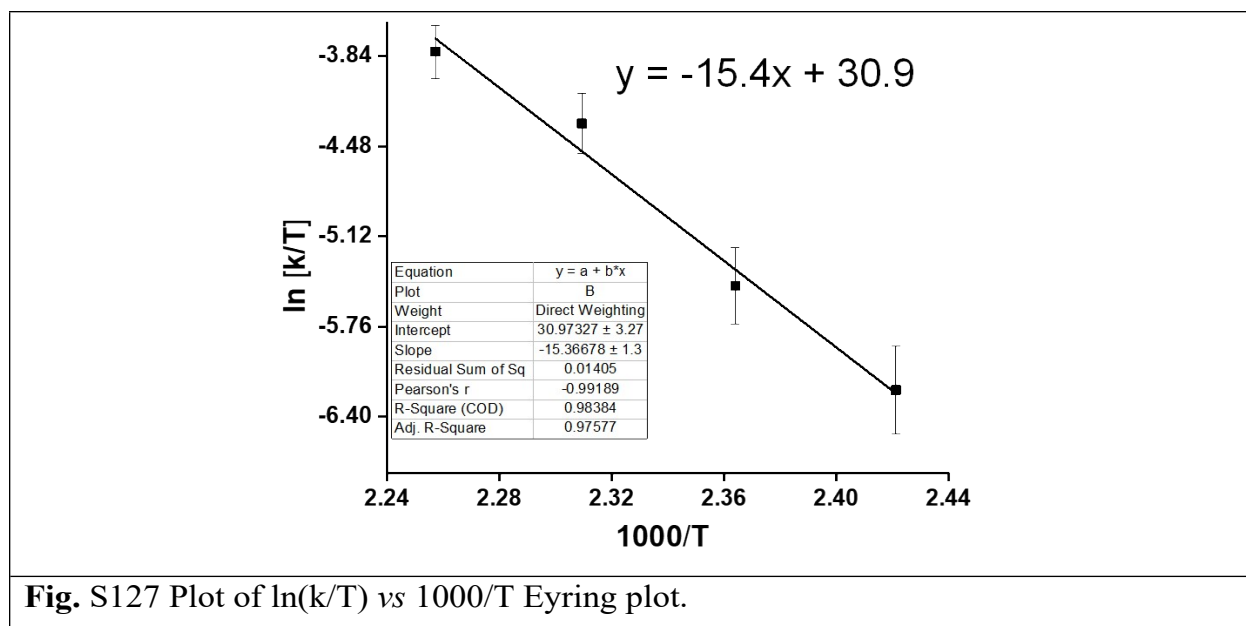
**Fig. S124** Plot of Conversion (%) vs time (h) at 423 K.



**Fig. S125** Plot of Conversion (%) vs time (h) at 433 K.



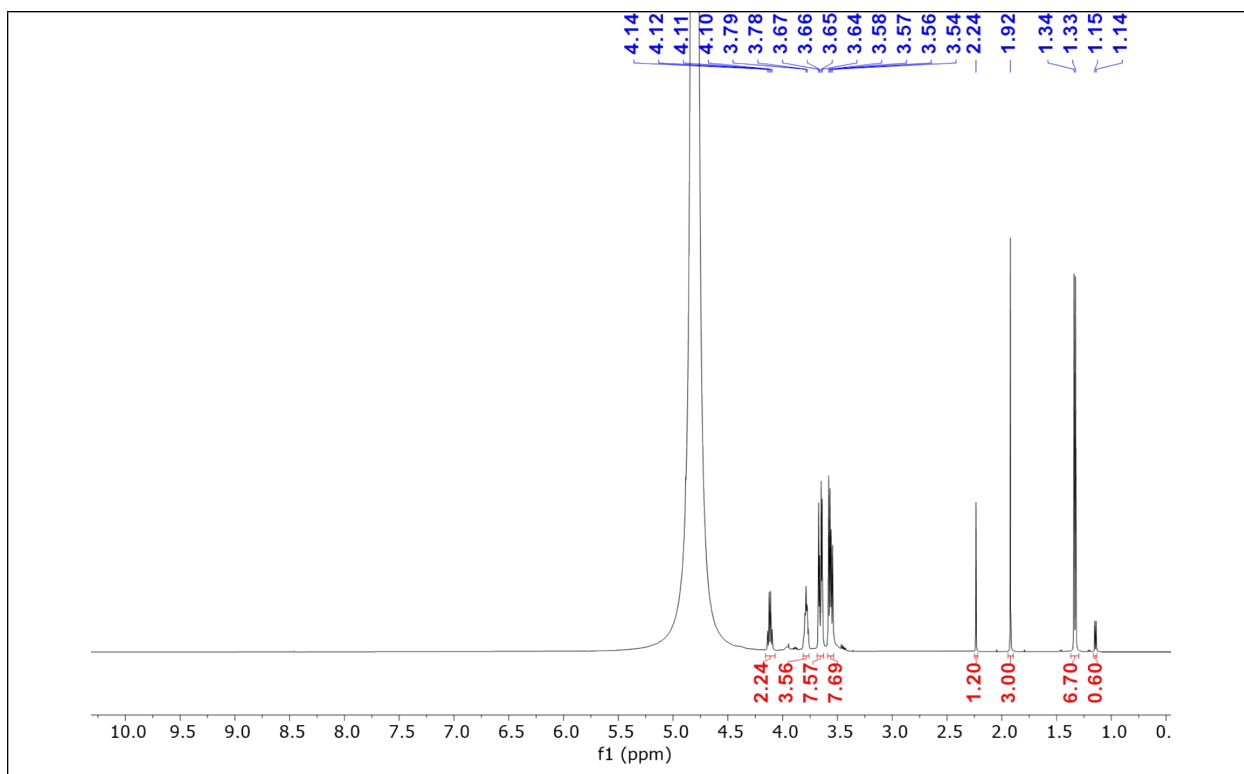
**Fig. S126** Plot of Conversion (%) vs time (h) at 443 K.



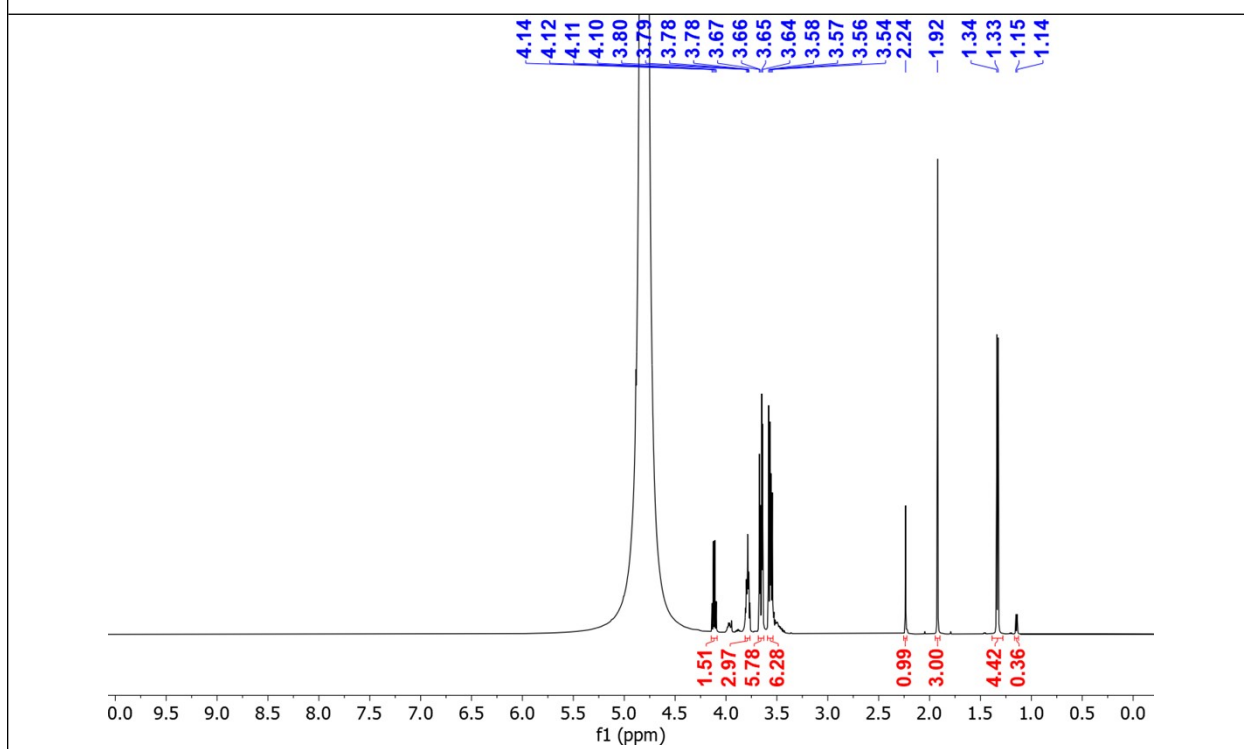
**Fig. S127** Plot of  $\ln(k/T)$  vs  $1000/T$  Eyring plot.

### 6.3 Mercury drop experiment

For this, glycerol (7 mmol; 0.510 mL), water (0.5 mL), NaOH (7 mmol; 0.280 g), **Ru-1** (0.05 mol%, 2.5 mg), and droplets of mercury were placed in a 20 mL glass tube and heated at 160 °C for 5 h. The conversion of glycerol was determined through  $^1\text{H}$  NMR spectroscopy in  $\text{D}_2\text{O}$  solvent, using KOAc as an external standard.



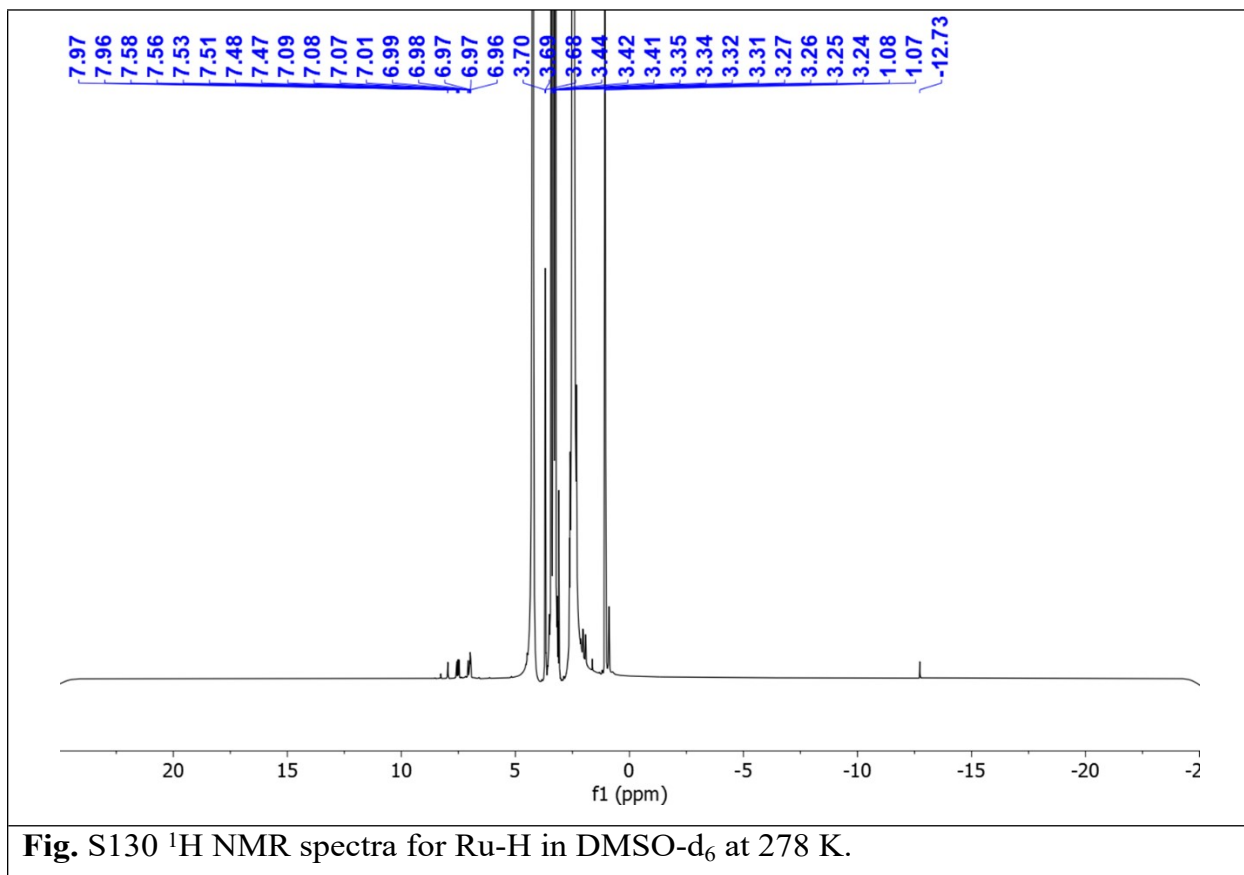
**Fig. S128**  $^1\text{H}$  NMR spectra for Glycerol to lactic acid (LA) with Hg droplet.



**Fig. S129**  $^1\text{H}$  NMR spectra for Glycerol to lactic acid (LA) without Hg droplet.

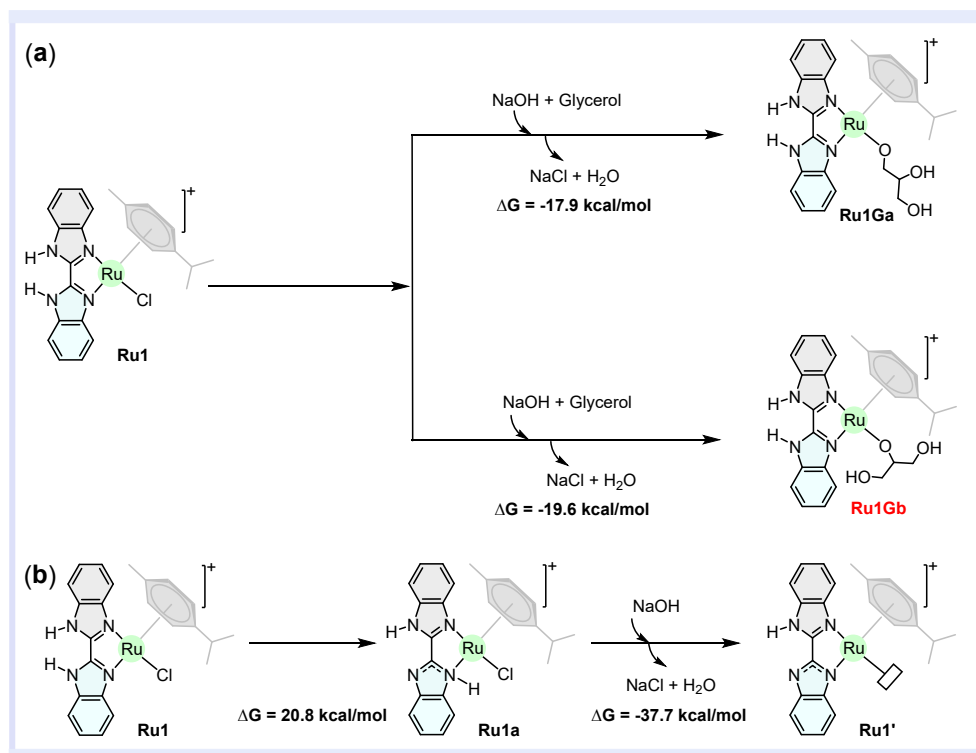
#### 6.4 Determination of Ru-H through $^1\text{H}$ NMR titration

For this, an NMR tube was charged with **Ru-1** (0.02 mmol), glycerol (0.1 mL),  $\text{H}_2\text{O}$  (0.2 mL), NaOH (0.4 mmol) and  $\text{DMSO-d}_6$  (0.5 mL) and was then heated in an oil bath at 125  $^\circ\text{C}$  for 1.5 h. The NMR tube was cooled and was put into the NMR probe.  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO-d}_6$ )  $\delta$  -12.73.



**Fig. S130**  $^1\text{H}$  NMR spectra for Ru-H in  $\text{DMSO-d}_6$  at 278 K.

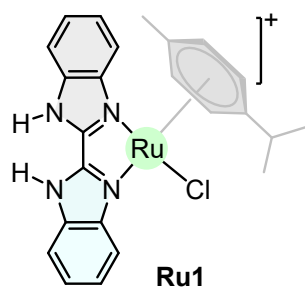
#### 6.5 Computational details<sup>1</sup>



**Scheme S1.** (a) DFT calculations for the coordination of primary and secondary hydroxyl groups of glycerol to **Ru-1**; (b) DFT calculation for base-assisted activation of the **Ru-1**.

The electronic energies, Gibbs free energies and the corresponding Cartesian coordinates of the species involved in the Catalytic mechanism are provided below:

**Ru-1**



**E sol -1700.850440**

**Gsol -1700.484348**

44 -1.383148000 -1.756578000 -  
0.396880000

17	-0.021556000	-0.710075000	-
	2.143282000		
6	-0.533546000	-3.774938000	-
	1.000991000		
6	-0.061070000	-3.421291000	
	0.302177000		
1	1.011646000	-3.378822000	
	0.493275000		
6	-0.986111000	-3.053313000	
	1.322607000		
1	-0.603361000	-2.710501000	
	2.287306000		
6	-2.402931000	-3.046461000	
	1.109190000		
6	-2.848036000	-3.376797000	-
	0.208655000		
1	-3.908425000	-3.287895000	-
	0.451364000		
6	-1.939056000	-3.754786000	-
	1.245398000		
1	-2.312712000	-3.976548000	-
	2.245406000		
6	0.429695000	-4.130598000	-
	2.090575000		
1	1.381412000	-3.596397000	-
	1.972720000		
1	0.015109000	-3.908330000	-
	3.082287000		
1	0.634039000	-5.213496000	-
	2.036531000		
6	-3.341454000	-2.687258000	
	2.242915000		
1	-2.794364000	-1.978286000	
	2.889038000		

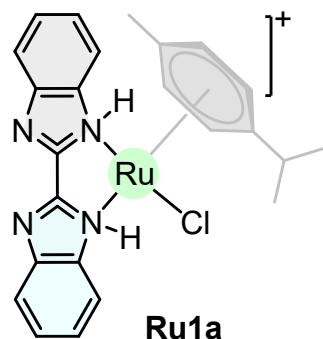
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	3.067943000		
1	-4.262649000	-3.709107000	
	3.934993000		
1	-2.704658000	-4.421141000	
	3.438298000		
1	-4.167247000	-4.702906000	
	2.456569000		
6	-4.640255000	-2.010784000	
	1.786365000		
1	-4.439207000	-1.126838000	
	1.163668000		
1	-5.215449000	-1.685422000	
	2.665710000		
1	-5.281614000	-2.699542000	
	1.213559000		
6	-5.474489000	-0.988519000	-
	3.582199000		
6	-6.096389000	0.279545000	-
	3.484515000		
6	-5.635727000	1.257733000	-
	2.602633000		
6	-4.529934000	0.918195000	-
	1.814931000		
6	-3.905806000	-0.359244000	-
	1.893845000		
6	-4.375842000	-1.327314000	-
	2.794645000		
1	-5.864995000	-1.717114000	-
	4.295201000		
1	-6.956050000	0.500170000	-
	4.120215000		
1	-6.108088000	2.238510000	-
	2.530613000		

1	-3.888045000	-2.297906000	-
	2.881849000		
6	-2.828887000	0.824623000	-
	0.395285000		
7	-2.860709000	-0.385292000	-
	0.986812000		
7	-3.821007000	1.632252000	-
	0.860880000		
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	1.978071000		
6	-1.771846000	1.019210000	
	0.547983000		
6	0.592481000	2.417035000	
	2.870144000		
6	0.045622000	0.374804000	
	1.589987000		
6	1.708150000	1.735208000	
	3.357039000		
1	0.372840000	3.444704000	
	3.162771000		
6	1.181362000	-0.290359000	
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6	2.000923000	0.407476000	
	2.962792000		
1	2.378087000	2.242672000	
	4.053782000		
1	1.420241000	-1.304618000	
	1.758211000		
1	2.894169000	-0.078799000	
	3.359454000		
7	-0.945756000	-0.031152000	
	0.713979000		
7	-1.379809000	2.084998000	
	1.298863000		

1 -4.010755000 2.588542000 -  
0.568518000

1 -1.843545000 2.989289000  
1.354387000

**Ru-1a**



**Esol : -1700.816052**

**Gsol : -1700.451208**

44	-1.233263000	-1.825869000	-0.491811000
17	0.582581000	-0.994433000	-1.912303000
6	-1.021022000	-3.930300000	-1.251367000
6	-0.241934000	-3.725988000	-0.051764000
1	0.837086000	-3.887738000	-0.078472000
6	-0.841381000	-3.235115000	1.135139000
1	-0.214125000	-3.040367000	2.007044000
6	-2.241126000	-2.883833000	1.185938000
6	-2.995464000	-3.053740000	-0.006598000
1	-4.032387000	-2.717174000	-0.047887000
6	-2.392344000	-3.578638000	-1.201709000
1	-2.986929000	-3.623334000	-2.116219000
6	-0.374218000	-4.419397000	-2.510319000

1	0.620457000	-3.969970000	-2.638949000
1	-0.987206000	-4.185092000	-3.390801000
1	-0.249533000	-5.513489000	-2.454583000
6	-2.822531000	-2.340269000	2.474184000
1	-2.043228000	-1.701507000	2.927187000
6	-3.077241000	-3.525293000	3.430808000
1	-3.438671000	-3.150060000	4.400035000
1	-2.161879000	-4.109520000	3.609259000
1	-3.841735000	-4.200460000	3.014668000
6	-4.087818000	-1.496437000	2.286237000
1	-3.936135000	-0.675998000	1.569089000
1	-4.378281000	-1.051126000	3.248861000
1	-4.935735000	-2.106980000	1.937377000
6	-5.029679000	-1.019728000	-4.149672000
6	-6.033001000	-0.213760000	-3.574955000
6	-5.791908000	0.547518000	-2.425914000
6	-4.512000000	0.472849000	-1.863436000
6	-3.523229000	-0.359009000	-2.439873000
6	-3.745765000	-1.106296000	-3.590545000
1	-5.256427000	-1.595051000	-5.049324000
1	-7.019725000	-0.181421000	-4.041153000
1	-6.561863000	1.181556000	-1.983389000
1	-2.967465000	-1.728979000	-4.034581000
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7	-2.358521000	-0.218362000	-1.628701000
7	-4.006558000	1.134084000	-0.731214000
6	-0.578673000	1.621265000	2.133184000

6	-1.811266000	0.925374000	0.430363000
6	0.028027000	2.304143000	3.194069000
6	-0.110197000	0.352691000	1.683832000
6	1.122132000	1.678650000	3.791543000
1	-0.337247000	3.274908000	3.531809000
6	0.998740000	-0.258155000	2.289816000
6	1.601779000	0.422614000	3.344896000
1	1.626648000	2.173378000	4.623711000
1	1.377286000	-1.216408000	1.932256000
1	2.469208000	-0.019045000	3.839055000
7	-0.913538000	-0.052965000	0.631970000
7	-1.653270000	1.941090000	1.317309000
1	-2.207088000	2.795424000	1.342088000
1	-1.472336000	0.011295000	-2.126427000

## H<sub>2</sub>O

**ESol : -76.380337**

**Gsol: -76.377959**

8	-0.813200000	-1.170845000
	-1.003340000	
1	-0.535551000	-1.138357000
	-0.073006000	
1	-1.783379000	-1.169134000
	-0.954349000	

**NaCl**

**Esol -622.332051**

**Gsol -622.354674**

11 -2.165707000 -1.474884000  
1.080449000

17 -4.863895000 -1.474884000  
1.080449000

**NaOH**

**Esol : -238.014694**

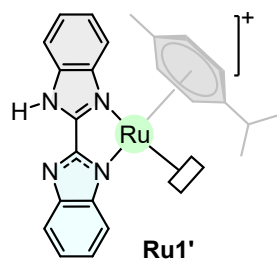
**Gsol : -238.027943**

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8 -4.324700000 -1.351879000 1.084745000

1 -4.927803000 -0.593539000 1.111227000

**Ru1'(deprotonated)**



**Esol -1240.161174**

**Gsol -1239.806564**

6	-5.346384000	-3.246596000	-
	2.412693000		
6	-4.115367000	-3.865984000	-
	2.806879000		
1	-4.147731000	-4.788818000	-
	3.387950000		
6	-2.885137000	-3.200053000	-
	2.603063000		
1	-1.968305000	-3.611533000	-
	3.030277000		
6	-2.832017000	-1.901347000	-
	1.982439000		
6	-4.058864000	-1.359692000	-
	1.455990000		
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	0.998603000		
6	-5.292507000	-2.017574000	-
	1.667693000		
1	-6.225608000	-1.531621000	-
	1.377955000		
6	-6.663953000	-3.870827000	-
	2.754841000		
1	-7.449485000	-3.111352000	-
	2.867776000		
1	-6.962827000	-4.546077000	-
	1.934150000		
1	-6.599350000	-4.465856000	-
	3.675710000		
6	-1.508035000	-1.179498000	-
	1.851919000		
1	-0.861984000	-1.564369000	-
	2.659821000		
6	-0.870242000	-1.570109000	-

0.500657000

1 0.124917000 -1.108266000 -  
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0.407246000

1 -1.487200000 -1.215442000  
0.340327000

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2.012780000

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1.179269000

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3.606016000

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7.305754000

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8.530697000

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9.345452000

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9.670861000

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5.292401000

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6.246805000

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5.555247000

7 -3.117676000 -0.800311000 -  
7.495537000

6 -5.135302000 2.227089000 -  
4.928034000

6 -4.278430000 0.391556000 -  
5.581780000

6 -5.625892000 3.537125000 -  
4.797780000

6 -5.228262000 1.300786000 -  
3.837916000

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3.442365000

1 -5.899261000 0.969786000 -  
1.787032000

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1.567343000

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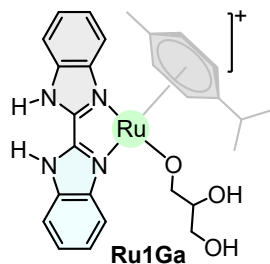
### **Glycerol**

**Esol -344.515158**

**Gsol -344.432291**

6	-1.011737000	-0.700513000	-0.130776000
1	-0.721942000	-0.871649000	-1.183469000
1	-0.947247000	-1.665093000	0.408534000
6	-0.042843000	0.289989000	0.515116000
1	-0.424468000	0.538968000	1.519845000
6	1.358934000	-0.298900000	0.663909000
1	1.320191000	-1.252823000	1.220830000
8	-2.339318000	-0.158066000	-0.043352000
1	-2.927733000	-0.736852000	-0.555148000
8	0.016545000	1.532353000	-0.206585000
1	0.596318000	1.358496000	-0.973012000
8	1.878277000	-0.498047000	-0.667369000
1	1.988200000	0.413544000	1.223350000
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### **Ru1Ga**



**Esol -1584.698765**

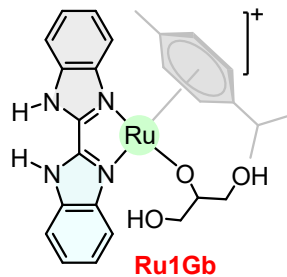
**Gsol -1584.240499**

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6	-0.295572000	-3.421946000	0.013391000
1	0.791657000	-3.349620000	0.064676000
6	-1.094170000	-3.029838000	1.134277000
1	-0.597548000	-2.637163000	2.025379000
6	-2.522251000	-3.103434000	1.128969000
6	-3.120612000	-3.487712000	-0.107470000
1	-4.207327000	-3.453121000	-0.207733000
6	-2.344263000	-3.886383000	-1.244535000
1	-2.842881000	-4.170982000	-2.172087000
6	-0.109884000	-4.174398000	-2.415637000
1	0.917126000	-4.461299000	-2.152086000
1	-0.064980000	-3.273431000	-3.053759000
1	-0.572620000	-4.983780000	-2.997999000
6	-3.323606000	-2.746842000	2.365481000
1	-2.668571000	-2.116247000	2.992059000
6	-3.639869000	-4.034930000	3.152745000

1	-4.164452000	-3.790479000	4.089376000
1	-2.721746000	-4.586882000	3.405735000
1	-4.288261000	-4.701514000	2.560859000
6	-4.599268000	-1.947554000	2.063543000
1	-4.374221000	-1.038277000	1.486707000
1	-5.082686000	-1.648289000	3.005714000
1	-5.331930000	-2.542831000	1.495571000
6	-6.286879000	-1.333050000	-3.189427000
6	-6.853362000	-0.036036000	-3.179646000
6	-6.244027000	1.025159000	-2.508686000
6	-5.047599000	0.739240000	-1.841796000
6	-4.474615000	-0.565018000	-1.831192000
6	-5.096384000	-1.617151000	-2.522050000
1	-6.793900000	-2.129200000	-3.738039000
1	-7.787768000	0.140558000	-3.715987000
1	-6.672247000	2.028589000	-2.506388000
1	-4.655368000	-2.613150000	-2.547093000
6	-3.159041000	0.754637000	-0.680640000
7	-3.308785000	-0.521232000	-1.085417000
7	-4.189082000	1.539585000	-1.104575000
6	-0.291013000	1.844111000	1.261371000
6	-1.983175000	1.029438000	0.081020000
6	0.627978000	2.618681000	1.978115000
6	-0.087690000	0.455543000	1.020483000
6	1.769658000	1.963408000	2.442015000
1	0.460643000	3.681385000	2.158915000
6	1.074216000	-0.183082000	1.480614000

6	1.991300000	0.588026000	2.193145000
1	2.514497000	2.528724000	3.005543000
1	1.257966000	-1.236493000	1.270597000
1	2.906079000	0.122024000	2.564434000
7	-1.166305000	-0.021698000	0.291833000
7	-1.494236000	2.166415000	0.651686000
1	-4.309104000	2.533016000	-0.921151000
1	-1.934208000	3.083888000	0.643232000
8	-0.927117000	-1.071750000	-2.330342000
6	0.408581000	-0.647658000	-2.290720000
1	0.550794000	0.267715000	-1.674129000
1	1.093520000	-1.418210000	-1.870548000
6	0.907737000	-0.312114000	-3.699407000
1	1.906423000	0.161519000	-3.590329000
6	-0.016482000	0.662769000	-4.417037000
1	-0.081960000	1.606867000	-3.845015000
1	-1.022073000	0.219167000	-4.496249000
8	1.042170000	-1.523423000	-4.467756000
1	1.108732000	-1.230488000	-5.396792000
8	0.550029000	0.891109000	-5.727139000
1	-0.158075000	1.209211000	-6.310165000

**Ru1Gb**



**Esol : -1584.703616**

**Gsol: -1584.243098**

44	-1.302080000	-1.784838000	-0.209713000
6	-0.415542000	-3.829299000	-0.692799000
6	-0.052257000	-3.437214000	0.629687000
1	1.000973000	-3.395818000	0.910374000
6	-1.062058000	-3.041256000	1.565867000
1	-0.755542000	-2.679039000	2.550503000
6	-2.456648000	-3.055707000	1.251194000
6	-2.790098000	-3.390877000	-0.096952000
1	-3.826689000	-3.307244000	-0.429128000
6	-1.798603000	-3.790205000	-1.051593000
1	-2.093347000	-4.022934000	-2.075768000
6	0.633809000	-4.079608000	-1.729601000
1	1.548448000	-4.490874000	-1.281316000
1	0.877484000	-3.102988000	-2.192100000
1	0.269714000	-4.758748000	-2.512487000
6	-3.484058000	-2.687068000	2.302902000
1	-2.976634000	-2.007168000	3.010101000
6	-3.891887000	-3.958427000	3.075714000

1	-4.588116000	-3.701978000	3.889103000
1	-3.016585000	-4.459540000	3.516528000
1	-4.395781000	-4.674138000	2.405879000
6	-4.712123000	-1.957400000	1.742621000
1	-4.422914000	-1.068151000	1.163291000
1	-5.359629000	-1.632094000	2.570535000
1	-5.316476000	-2.611324000	1.093737000
6	-5.043620000	-0.959960000	-3.779100000
6	-5.624312000	0.331149000	-3.772919000
6	-5.228124000	1.311708000	-2.862460000
6	-4.227485000	0.952062000	-1.952614000
6	-3.644741000	-0.347189000	-1.942202000
6	-4.050394000	-1.319263000	-2.869904000
1	-5.381804000	-1.689868000	-4.517078000
1	-6.400459000	0.567913000	-4.503287000
1	-5.670150000	2.309097000	-2.862414000
1	-3.593206000	-2.308764000	-2.883005000
6	-2.680524000	0.832791000	-0.367633000
7	-2.694604000	-0.387853000	-0.937214000
7	-3.594921000	1.662640000	-0.943665000
6	-0.321272000	1.695657000	2.256534000
6	-1.706480000	1.017885000	0.663165000
6	0.402397000	2.384246000	3.236867000
6	-0.016179000	0.354328000	1.889749000
6	1.452252000	1.690589000	3.839807000
1	0.159015000	3.411872000	3.510637000
6	1.051210000	-0.324132000	2.499377000

6	1.773456000	0.361287000	3.474586000
1	2.045077000	2.188555000	4.609496000
1	1.312634000	-1.341161000	2.207028000
1	2.610885000	-0.136776000	3.966926000
7	-0.900677000	-0.038117000	0.897132000
7	-1.391375000	2.075781000	1.460723000
1	-3.771841000	2.633619000	-0.695322000
1	-1.857196000	2.980598000	1.478420000
8	-0.139365000	-1.139818000	-1.814490000
6	0.463301000	0.125907000	-1.931474000
1	-0.138041000	0.923838000	-1.443021000
6	0.469282000	0.450885000	-3.438793000
1	0.735695000	1.505457000	-3.612325000
1	1.207974000	-0.189842000	-3.963649000
6	1.860244000	0.200065000	-1.295102000
1	2.262747000	1.225109000	-1.424080000
1	1.769313000	0.009990000	-0.216072000
8	-0.839856000	0.220239000	-3.974275000
1	-1.142532000	-0.548246000	-3.437300000
8	2.794503000	-0.781399000	-1.775185000
1	2.949074000	-0.613967000	-2.719817000

## **Byproduct 2**

**Esol -343.312445**

**Gsol -343.253417**

6	-1.023534000	-0.703478000	-0.118010000
1	-0.694911000	-0.901367000	-1.156495000
1	-0.994589000	-1.661268000	0.440317000
6	-0.043077000	0.271167000	0.534933000
6	1.357049000	-0.329627000	0.657627000
1	1.326789000	-1.306611000	1.175487000
8	-2.328357000	-0.115825000	-0.076973000
1	-2.925130000	-0.723628000	-0.542221000
8	0.035387000	1.510190000	-0.182636000
8	1.855595000	-0.467419000	-0.688622000
1	1.988833000	0.361819000	1.240687000
1	2.824186000	-0.437073000	-0.648338000

### **Byproduct 1**

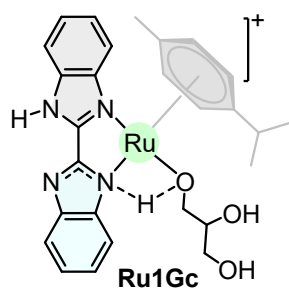
**Esol -343.312463**

**Gsol -343.252331**

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6	1.357049000	-0.329627000	0.657627000
1	1.326789000	-1.306611000	1.175487000
8	-2.410011430	-0.366557470	-0.213219670
8	0.035387000	1.510190000	-0.182636000

8	1.855595000	-0.467419000	-0.688622000
1	1.988833000	0.361819000	1.240687000
1	2.824186000	-0.437073000	-0.648338000
1	0.956637580	1.743831260	-0.317947230
1	-0.398387750	0.483519550	1.521624780
1	-0.672268110	-1.637680150	-0.503728320

### Ru1Gc



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**Gsol : -1584.241424**

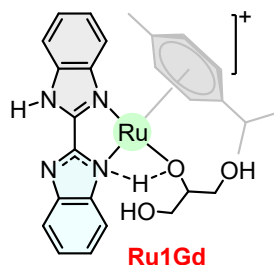
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6	-3.915989000	-3.442889000	-3.139130000
1	-3.684684000	-4.048958000	-4.017907000
6	-3.156529000	-2.269247000	-2.886846000
1	-2.350913000	-2.002649000	-3.574766000
6	-3.468986000	-1.387219000	-1.786351000
6	-4.606546000	-1.704784000	-1.005061000
1	-4.947034000	-1.016988000	-0.231000000
6	-5.388536000	-2.882061000	-1.279768000

1	-6.303670000	-3.052796000	-0.707611000
6	-5.873638000	-5.000774000	-2.632964000
1	-6.808066000	-5.011477000	-2.055824000
1	-5.309820000	-5.916911000	-2.393925000
1	-6.114924000	-5.024059000	-3.706964000
6	-2.590978000	-0.173520000	-1.548239000
1	-2.469251000	0.328944000	-2.525491000
6	-1.196700000	-0.657647000	-1.092423000
1	-0.524405000	0.205076000	-0.971351000
1	-0.740273000	-1.345951000	-1.819381000
1	-1.266934000	-1.177841000	-0.123778000
6	-3.165314000	0.837103000	-0.551106000
1	-4.164311000	1.187245000	-0.846988000
1	-2.506090000	1.716155000	-0.498289000
1	-3.227671000	0.408423000	0.462264000
44	-5.245544000	-1.741513000	-3.163143000
6	-7.267150000	-1.605956000	-5.254403000
6	-8.154148000	-1.315634000	-4.051736000
8	-6.207368000	-2.459239000	-4.857831000
1	-7.860340000	-2.105861000	-6.042679000
1	-8.861730000	-0.496394000	-4.259678000
6	-2.478325000	-4.721618000	-8.616919000
6	-1.411427000	-3.885964000	-9.034283000
6	-1.266911000	-2.586547000	-8.549249000
6	-2.222413000	-2.121830000	-7.624806000
6	-3.290345000	-2.979104000	-7.211502000
6	-3.435870000	-4.286462000	-7.699467000

1	-2.550399000	-5.732797000	-9.023849000
1	-0.686979000	-4.274254000	-9.753809000
1	-0.444180000	-1.944454000	-8.871366000
1	-4.256043000	-4.930304000	-7.375958000
6	-3.411556000	-1.021049000	-6.218377000
7	-4.029441000	-2.241122000	-6.314374000
7	-2.325514000	-0.897205000	-6.989163000
6	-4.176882000	2.180543000	-4.754987000
6	-3.910173000	0.060455000	-5.392830000
6	-4.152659000	3.570207000	-4.587166000
6	-4.939922000	1.321427000	-3.919551000
6	-4.925817000	4.087213000	-3.546892000
1	-3.558547000	4.211956000	-5.239543000
6	-5.711121000	1.860162000	-2.876821000
6	-5.692013000	3.244952000	-2.708330000
1	-4.940212000	5.165847000	-3.377839000
1	-6.309169000	1.215217000	-2.235421000
1	-6.284246000	3.690473000	-1.906325000
7	-4.740776000	-0.000036000	-4.333544000
7	-3.549041000	1.349612000	-5.660769000
1	-4.952988000	-2.465107000	-5.824911000
1	-2.931990000	1.611944000	-6.427710000
1	-6.896701000	-0.646760000	-5.664147000
6	-8.882655000	-2.548222000	-3.521133000
1	-9.756460000	-2.765320000	-4.157877000
1	-8.199555000	-3.411832000	-3.528606000
8	-9.289066000	-2.228796000	-2.172399000

1	-9.337522000	-3.052562000	-1.659632000
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1	-7.706796000	-1.106519000	-2.159945000

### Ru1Gd



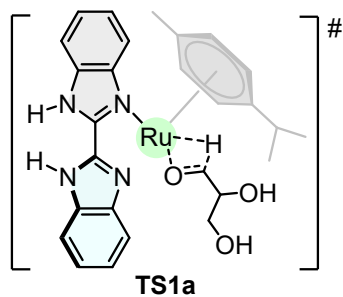
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**Gsol: -1584.220077**

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1	-4.789917000	-4.663480000	-2.682177000
6	-3.404228000	-2.971792000	-2.688013000
1	-2.825642000	-3.360995000	-3.529249000
6	-3.027930000	-1.703529000	-2.103841000
6	-3.853980000	-1.181091000	-1.068361000
1	-3.675195000	-0.180630000	-0.675082000
6	-5.029254000	-1.875226000	-0.679138000
1	-5.732336000	-1.385450000	-0.001572000
6	-6.619244000	-3.873626000	-0.755169000
1	-7.426568000	-3.149111000	-0.575822000
1	-6.431655000	-4.404281000	0.193396000

1	-6.956549000	-4.607272000	-1.499222000
6	-1.796423000	-0.994928000	-2.627194000
1	-1.790506000	-1.129580000	-3.723666000
6	-0.552635000	-1.720246000	-2.064690000
1	0.358913000	-1.261112000	-2.475822000
1	-0.547200000	-2.788455000	-2.328203000
1	-0.517780000	-1.634203000	-0.967225000
6	-1.741529000	0.505390000	-2.319453000
1	-2.646389000	1.033939000	-2.652362000
1	-0.879467000	0.953419000	-2.834653000
1	-1.613641000	0.690856000	-1.241065000
44	-5.111096000	-1.724874000	-2.869479000
6	-7.147904000	-1.769640000	-5.044345000
6	-8.455133000	-2.022440000	-4.270308000
8	-6.052230000	-2.491430000	-4.479815000
1	-6.966245000	-0.676649000	-4.993403000
1	-8.245687000	-1.926761000	-3.192646000
8	-9.007347000	-3.330091000	-4.467855000
1	-9.351946000	-3.336853000	-5.380011000
6	-1.835341000	-4.251162000	-8.221278000
6	-0.956801000	-3.242306000	-8.690971000
6	-1.053701000	-1.923344000	-8.249446000
6	-2.061458000	-1.619023000	-7.314387000
6	-2.933029000	-2.650440000	-6.846372000
6	-2.839313000	-3.976634000	-7.291332000
1	-1.721157000	-5.270524000	-8.596658000
1	-0.186069000	-3.509940000	-9.417223000

1	-0.376784000	-1.146985000	-8.612149000
1	-3.514635000	-4.752898000	-6.926980000
6	-3.408457000	-0.710331000	-5.909704000
7	-3.777388000	-2.033970000	-5.948422000
7	-2.384714000	-0.414297000	-6.713782000
6	-4.681429000	2.321358000	-4.426055000
6	-4.069349000	0.279664000	-5.084777000
6	-4.903502000	3.691794000	-4.246430000
6	-5.237585000	1.343206000	-3.559703000
6	-5.706015000	4.056836000	-3.164463000
1	-4.470693000	4.433300000	-4.919488000
6	-6.041629000	1.725953000	-2.475015000
6	-6.265566000	3.091092000	-2.295143000
1	-5.907897000	5.114747000	-2.985170000
1	-6.477741000	0.984425000	-1.803264000
1	-6.889198000	3.423847000	-1.463070000
7	-4.827739000	0.080578000	-3.990460000
7	-3.956405000	1.611316000	-5.363712000
1	-9.187885000	-1.244071000	-4.548675000
6	-7.253682000	-2.212159000	-6.512338000
1	-6.446432000	-1.749833000	-7.106335000
1	-7.127501000	-3.309636000	-6.548010000
8	-8.548619000	-1.828298000	-7.013076000
1	-8.597198000	-2.100376000	-7.944767000
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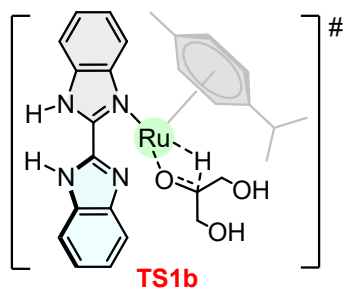
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1	-4.814785000	-4.826492000	-3.122804000
6	-3.457568000	-3.176605000	-2.669661000
1	-2.669692000	-3.549379000	-3.324213000
6	-3.300578000	-1.916772000	-2.046722000
6	-4.418992000	-1.384642000	-1.306984000
1	-4.358026000	-0.390619000	-0.865451000
6	-5.609519000	-2.142877000	-1.144939000
1	-6.442839000	-1.711991000	-0.585797000
6	-6.985455000	-4.272361000	-1.501146000
1	-7.882678000	-3.652752000	-1.366215000
1	-6.842581000	-4.851514000	-0.573542000
1	-7.158732000	-4.988340000	-2.315758000
6	-1.987769000	-1.172754000	-2.191878000
1	-1.674877000	-1.321322000	-3.239813000

6	-0.944788000	-1.845825000	-1.271824000
1	0.032386000	-1.354883000	-1.397604000
1	-0.825424000	-2.914189000	-1.506287000
1	-1.239280000	-1.755613000	-0.213686000
6	-2.069612000	0.332354000	-1.910624000
1	-2.835686000	0.827415000	-2.524612000
1	-1.100348000	0.799131000	-2.140751000
1	-2.288439000	0.540200000	-0.850642000
44	-5.234656000	-1.865278000	-3.309130000
1	-7.037306000	-0.904229000	-5.342384000
6	-6.805239000	-1.891042000	-4.889084000
6	-8.050572000	-2.749677000	-4.682043000
8	-5.690860000	-2.473686000	-5.288319000
1	-6.720640000	-1.194168000	-3.434050000
1	-7.754747000	-3.708365000	-4.217561000
8	-8.566786000	-2.984076000	-6.002109000
1	-9.518163000	-3.173269000	-5.866399000
6	-9.110789000	-2.052414000	-3.830205000
1	-9.284300000	-1.031784000	-4.217133000
1	-8.779119000	-1.983494000	-2.779474000
8	-10.304276000	-2.847261000	-3.943460000
1	-11.068220000	-2.285098000	-3.734493000
6	-0.745655000	-4.277101000	-7.789556000
6	-1.196250000	-3.722625000	-9.012871000
6	-2.034874000	-2.606495000	-9.050206000
6	-2.407073000	-2.065419000	-7.812823000
6	-1.971924000	-2.615106000	-6.571766000

6	-1.121869000	-3.736495000	-6.560250000
1	-0.089265000	-5.149752000	-7.814793000
1	-0.877698000	-4.179408000	-9.952450000
1	-2.378805000	-2.178802000	-9.993676000
1	-0.776625000	-4.163617000	-5.616307000
6	-3.234890000	-0.946389000	-6.082135000
7	-2.499690000	-1.892521000	-5.513969000
7	-3.198906000	-0.987803000	-7.463257000
6	-4.728758000	2.134997000	-4.884425000
6	-3.967100000	0.089816000	-5.368337000
6	-5.046556000	3.496927000	-4.823939000
6	-5.192787000	1.203350000	-3.922113000
6	-5.858387000	3.900264000	-3.762995000
1	-4.679164000	4.203584000	-5.569488000
6	-6.016285000	1.622201000	-2.865954000
6	-6.337461000	2.977935000	-2.803142000
1	-6.132814000	4.953202000	-3.673364000
1	-6.388535000	0.909564000	-2.128963000
1	-6.974388000	3.337745000	-1.992669000
7	-4.702472000	-0.059895000	-4.253924000
7	-3.974251000	1.395504000	-5.778078000
1	-3.764018000	-0.429807000	-8.099743000
1	-3.413389000	1.770824000	-6.540859000

**TS1b**



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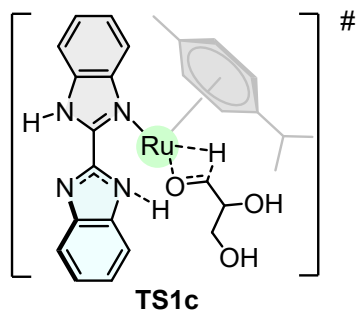
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6	-3.547680000	-3.168952000	-2.654264000
1	-2.770340000	-3.599025000	-3.286547000
6	-3.341150000	-1.898961000	-2.071929000
6	-4.446974000	-1.294247000	-1.366451000
1	-4.350781000	-0.285762000	-0.965261000
6	-5.665176000	-1.997344000	-1.177294000
1	-6.481097000	-1.516422000	-0.633864000
6	-7.115152000	-4.081544000	-1.441078000
1	-7.997619000	-3.427517000	-1.405569000
1	-7.015128000	-4.556850000	-0.450930000
1	-7.284809000	-4.878260000	-2.176798000
6	-1.994668000	-1.216954000	-2.220907000
1	-1.688040000	-1.386642000	-3.267415000
6	-0.982284000	-1.928599000	-1.295895000
1	0.016021000	-1.482853000	-1.424542000

1	-0.910379000	-3.002857000	-1.522518000
1	-1.272442000	-1.818090000	-0.238447000
6	-2.007059000	0.292148000	-1.949001000
1	-2.747236000	0.820453000	-2.567106000
1	-1.016552000	0.712229000	-2.178574000
1	-2.219384000	0.515676000	-0.890793000
44	-5.272796000	-1.808365000	-3.348799000
6	-6.860383000	-1.980004000	-4.967599000
6	-7.930437000	-3.023962000	-4.586415000
8	-5.673608000	-2.402347000	-5.356384000
1	-6.766659000	-1.161047000	-3.557131000
1	-7.414644000	-3.964864000	-4.353998000
8	-8.801315000	-3.284016000	-5.694333000
1	-9.378203000	-2.500138000	-5.772411000
6	-0.816825000	-4.262478000	-7.842630000
6	-1.150750000	-3.598391000	-9.048819000
6	-1.904998000	-2.423089000	-9.057512000
6	-2.314699000	-1.936964000	-7.809174000
6	-1.996202000	-2.595815000	-6.585745000
6	-1.229767000	-3.775959000	-6.602672000
1	-0.223604000	-5.178335000	-7.890380000
1	-0.807400000	-4.016267000	-9.997726000
1	-2.159640000	-1.911676000	-9.987525000
1	-0.975472000	-4.287715000	-5.672060000
6	-3.170705000	-0.875807000	-6.055059000
7	-2.538058000	-1.907442000	-5.513196000
7	-3.052189000	-0.830717000	-7.432406000

6	-4.592904000	2.214080000	-4.794584000
6	-3.883672000	0.159062000	-5.321139000
6	-4.864055000	3.584009000	-4.696695000
6	-5.138457000	1.265437000	-3.893622000
6	-5.716957000	3.976924000	-3.664640000
1	-4.432716000	4.303699000	-5.393926000
6	-6.005090000	1.674297000	-2.868328000
6	-6.281241000	3.037568000	-2.769524000
1	-5.958466000	5.035274000	-3.547993000
1	-6.444980000	0.947064000	-2.184991000
1	-6.950297000	3.390177000	-1.982130000
7	-4.680045000	-0.003123000	-4.250484000
7	-3.822700000	1.479706000	-5.678762000
1	-3.533387000	-0.191384000	-8.061480000
1	-3.207897000	1.862585000	-6.394427000
1	-8.505112000	-2.695875000	-3.705403000
6	-7.413105000	-0.777474000	-5.736743000
1	-6.700010000	0.057982000	-5.714889000
1	-7.524070000	-1.110051000	-6.785853000
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**TS1c**



**Esol : -1584.667284**

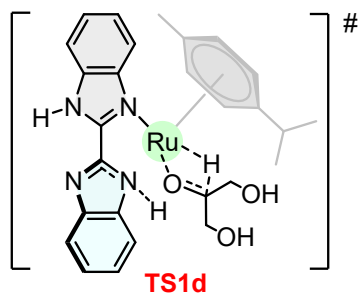
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6	-3.434686000	-3.201718000	-2.681598000
1	-2.677803000	-3.669823000	-3.314054000
6	-3.255434000	-1.869089000	-2.248146000
6	-4.335719000	-1.248509000	-1.516831000
1	-4.265688000	-0.201309000	-1.224628000
6	-5.499968000	-1.984774000	-1.171530000
1	-6.300409000	-1.486771000	-0.620792000
6	-6.876425000	-4.143943000	-1.167426000
1	-7.770389000	-3.512137000	-1.073221000
1	-6.679498000	-4.587935000	-0.177337000
1	-7.083545000	-4.966065000	-1.865385000
6	-1.956371000	-1.144950000	-2.552414000
1	-1.676825000	-1.408836000	-3.587549000
6	-0.863927000	-1.703324000	-1.611795000
1	0.100019000	-1.224276000	-1.840419000

1	-0.744809000	-2.790771000	-1.725802000
1	-1.112451000	-1.490544000	-0.559894000
6	-2.031952000	0.382595000	-2.439934000
1	-2.843959000	0.810436000	-3.044143000
1	-1.086205000	0.820659000	-2.790218000
1	-2.176720000	0.703717000	-1.396181000
44	-5.281393000	-1.997139000	-3.372128000
1	-7.127930000	-1.337802000	-5.427606000
6	-6.918548000	-2.260124000	-4.852382000
6	-8.166706000	-3.055036000	-4.487625000
8	-5.835428000	-2.939331000	-5.195453000
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1	-7.870630000	-3.930156000	-3.879866000
8	-8.710615000	-3.488424000	-5.742641000
1	-9.664366000	-3.625433000	-5.564994000
6	-9.199647000	-2.212698000	-3.736987000
1	-9.364007000	-1.260952000	-4.273887000
1	-8.848781000	-1.989565000	-2.713881000
8	-10.405648000	-2.994335000	-3.709368000
1	-11.158048000	-2.393286000	-3.582648000
6	-0.951954000	-4.320380000	-8.191120000
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6	-0.235524000	-1.991016000	-7.893488000
6	-1.448490000	-1.749423000	-7.220268000
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6	-2.159515000	-4.108121000	-7.524587000
1	-0.727558000	-5.315198000	-8.582320000

1	0.925995000	-3.499420000	-8.898128000
1	0.493867000	-1.190160000	-8.031732000
1	-2.886560000	-4.909746000	-7.383042000
6	-3.111317000	-0.936680000	-6.131807000
7	-3.437381000	-2.251443000	-6.347095000
7	-1.929865000	-0.585934000	-6.645213000
6	-4.765517000	2.022884000	-4.914098000
6	-3.968337000	0.005809000	-5.440150000
6	-5.068003000	3.384657000	-4.797644000
6	-5.416068000	1.027970000	-4.138444000
6	-6.049553000	3.728664000	-3.867857000
1	-4.559264000	4.134800000	-5.404722000
6	-6.395232000	1.392706000	-3.201098000
6	-6.701336000	2.748566000	-3.083797000
1	-6.319958000	4.778895000	-3.741973000
1	-6.896526000	0.642415000	-2.588278000
1	-7.461977000	3.061714000	-2.365974000
7	-4.890233000	-0.221205000	-4.482216000
7	-3.868178000	1.339047000	-5.710052000
1	-3.226967000	1.724286000	-6.402035000
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**TS1d**



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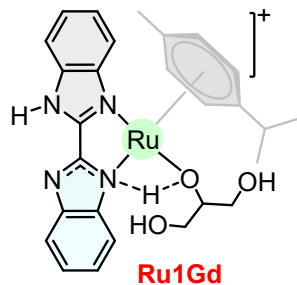
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6	-3.539786000	-3.151067000	-2.649348000
1	-2.817343000	-3.671088000	-3.281676000
6	-3.280952000	-1.826024000	-2.236779000
6	-4.319500000	-1.135425000	-1.505730000
1	-4.190594000	-0.087706000	-1.235425000
6	-5.513563000	-1.801039000	-1.124685000
1	-6.274506000	-1.253809000	-0.564968000
6	-6.985250000	-3.886100000	-1.030471000
1	-7.861088000	-3.223491000	-0.993978000
1	-6.799507000	-4.247006000	-0.005065000
1	-7.215473000	-4.759373000	-1.654259000
6	-1.945711000	-1.180122000	-2.564792000
1	-1.717113000	-1.430395000	-3.615731000
6	-0.861082000	-1.833895000	-1.678497000
1	0.123956000	-1.410537000	-1.926441000

1	-0.815181000	-2.922812000	-1.826138000
1	-1.061329000	-1.637337000	-0.613204000
6	-1.915860000	0.344869000	-2.406963000
1	-2.714097000	0.845742000	-2.972242000
1	-0.953740000	0.730701000	-2.773794000
1	-2.008641000	0.641409000	-1.350000000
44	-5.330713000	-1.858438000	-3.328809000
6	-7.040281000	-2.211311000	-4.783150000
6	-8.120955000	-3.144068000	-4.202047000
8	-5.901605000	-2.756128000	-5.177979000
1	-6.841155000	-1.242475000	-3.444283000
1	-7.629807000	-4.069822000	-3.875167000
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1	-9.635215000	-2.720394000	-5.347614000
6	-1.107453000	-4.235402000	-8.251677000
6	-0.115834000	-3.233184000	-8.402519000
6	-0.285334000	-1.951970000	-7.880115000
6	-1.483064000	-1.679287000	-7.191611000
6	-2.468623000	-2.703387000	-7.044190000
6	-2.301113000	-3.991944000	-7.570911000
1	-0.929960000	-5.225405000	-8.677602000
1	0.802220000	-3.476012000	-8.942226000
1	0.478715000	-1.180413000	-7.995835000
1	-3.062941000	-4.764386000	-7.451955000
6	-3.103181000	-0.829961000	-6.066116000
7	-3.488065000	-2.121255000	-6.322663000
7	-1.909132000	-0.515835000	-6.574781000

6	-4.600382000	2.168881000	-4.748492000
6	-3.910906000	0.129731000	-5.340251000
6	-4.831044000	3.540208000	-4.586597000
6	-5.308472000	1.184797000	-4.010581000
6	-5.801207000	3.903240000	-3.652062000
1	-4.278937000	4.282838000	-5.164324000
6	-6.278349000	1.567504000	-3.071189000
6	-6.512402000	2.932877000	-2.908252000
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1	-3.070194000	1.836225000	-6.238758000
1	-8.621151000	-2.673207000	-3.340949000
6	-7.580823000	-1.088889000	-5.663540000
1	-6.817285000	-0.312863000	-5.810834000
1	-7.800248000	-1.549506000	-6.645406000
8	-8.770445000	-0.576375000	-5.051072000
1	-9.102021000	0.153216000	-5.600842000
1	-4.415898000	-2.503697000	-6.072035000

**Ru1Gd**



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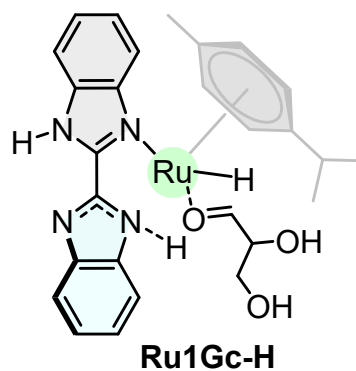
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6	-3.404228000	-2.971792000	-2.688013000
1	-2.825642000	-3.360995000	-3.529249000
6	-3.027930000	-1.703529000	-2.103841000
6	-3.853980000	-1.181091000	-1.068361000
1	-3.675195000	-0.180630000	-0.675082000
6	-5.029254000	-1.875226000	-0.679138000
1	-5.732336000	-1.385450000	-0.001572000
6	-6.619244000	-3.873626000	-0.755169000
1	-7.426568000	-3.149111000	-0.575822000
1	-6.431655000	-4.404281000	0.193396000
1	-6.956549000	-4.607272000	-1.499222000
6	-1.796423000	-0.994928000	-2.627194000
1	-1.790506000	-1.129580000	-3.723666000
6	-0.552635000	-1.720246000	-2.064690000

1	0.358913000	-1.261112000	-2.475822000
1	-0.547200000	-2.788455000	-2.328203000
1	-0.517780000	-1.634203000	-0.967225000
6	-1.741529000	0.505390000	-2.319453000
1	-2.646389000	1.033939000	-2.652362000
1	-0.879467000	0.953419000	-2.834653000
1	-1.613641000	0.690856000	-1.241065000
44	-5.111096000	-1.724874000	-2.869479000
6	-7.147904000	-1.769640000	-5.044345000
6	-8.455133000	-2.022440000	-4.270308000
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1	-8.245687000	-1.926761000	-3.192646000
8	-9.007347000	-3.330091000	-4.467855000
1	-9.351946000	-3.336853000	-5.380011000
6	-1.835341000	-4.251162000	-8.221278000
6	-0.956801000	-3.242306000	-8.690971000
6	-1.053701000	-1.923344000	-8.249446000
6	-2.061458000	-1.619023000	-7.314387000
6	-2.933029000	-2.650440000	-6.846372000
6	-2.839313000	-3.976634000	-7.291332000
1	-1.721157000	-5.270524000	-8.596658000
1	-0.186069000	-3.509940000	-9.417223000
1	-0.376784000	-1.146985000	-8.612149000
1	-3.514635000	-4.752898000	-6.926980000
6	-3.408457000	-0.710331000	-5.909704000
7	-3.777388000	-2.033970000	-5.948422000

7	-2.384714000	-0.414297000	-6.713782000
6	-4.681429000	2.321358000	-4.426055000
6	-4.069349000	0.279664000	-5.084777000
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6	-5.237585000	1.343206000	-3.559703000
6	-5.706015000	4.056836000	-3.164463000
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6	-6.265566000	3.091092000	-2.295143000
1	-5.907897000	5.114747000	-2.985170000
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1	-6.889198000	3.423847000	-1.463070000
7	-4.827739000	0.080578000	-3.990460000
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8	-8.548619000	-1.828298000	-7.013076000
1	-8.597198000	-2.100376000	-7.944767000
1	-4.625911000	-2.414944000	-5.468163000
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**Ru-1Gc-H**



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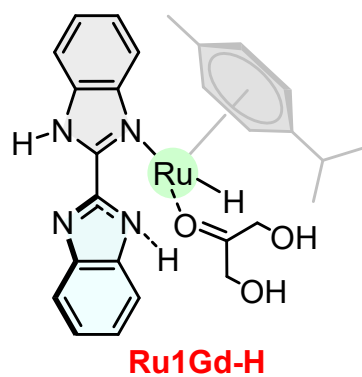
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6	1.183252000	-1.714890000	1.541988000
1	1.936858000	-2.195451000	0.914594000
6	1.387190000	-0.395695000	1.992353000
6	0.304520000	0.234203000	2.711747000
1	0.390102000	1.273394000	3.027205000
6	-0.854554000	-0.506939000	3.084438000
1	-1.632319000	-0.012014000	3.669374000
6	-2.230620000	-2.667050000	3.109419000
1	-3.115043000	-2.040382000	3.286800000
1	-1.972903000	-3.154836000	4.064304000
1	-2.483097000	-3.458665000	2.391454000
6	2.702014000	0.308913000	1.719015000
1	3.000203000	0.039860000	0.690435000
6	3.766851000	-0.264661000	2.682420000
1	4.741795000	0.200120000	2.471936000

1	3.871786000	-1.353781000	2.570607000
1	3.500521000	-0.047338000	3.728892000
6	2.641666000	1.837448000	1.827197000
1	1.845108000	2.271389000	1.206517000
1	3.598243000	2.264046000	1.492731000
1	2.481413000	2.163152000	2.867174000
44	-0.706929000	-0.446740000	0.866357000
1	-2.469452000	0.122106000	-1.171758000
6	-2.244071000	-0.813310000	-0.627648000
6	-3.463863000	-1.618533000	-0.222691000
8	-1.139491000	-1.450499000	-0.952799000
1	-2.041816000	0.360652000	1.136309000
1	-3.137565000	-2.518952000	0.329854000
8	-4.096345000	-2.006992000	-1.456326000
1	-5.037212000	-2.142853000	-1.217839000
6	-4.445086000	-0.803153000	0.621019000
1	-4.627177000	0.173799000	0.137989000
1	-4.033161000	-0.630346000	1.629550000
8	-5.659142000	-1.572514000	0.683620000
1	-6.396037000	-0.967901000	0.869857000
6	3.762702000	-2.774325000	-3.948680000
6	4.689714000	-1.715957000	-4.125456000
6	4.439945000	-0.435291000	-3.635160000
6	3.226293000	-0.221047000	-2.953861000
6	2.306970000	-1.300877000	-2.779454000
6	2.555777000	-2.589511000	-3.272935000
1	4.001723000	-3.761165000	-4.351211000

1	5.621029000	-1.913869000	-4.660764000
1	5.153410000	0.380021000	-3.771918000
1	1.843250000	-3.404733000	-3.135216000
6	1.548379000	0.556285000	-1.860126000
7	1.249437000	-0.764029000	-2.078167000
7	2.724085000	0.929784000	-2.373072000
6	-0.074579000	3.544740000	-0.692101000
6	0.678773000	1.502259000	-1.186256000
6	-0.333600000	4.916990000	-0.593441000
6	-0.767696000	2.575656000	0.079569000
6	-1.316624000	5.303401000	0.317083000
1	0.211001000	5.642810000	-1.199042000
6	-1.748293000	2.985753000	0.996913000
6	-2.011450000	4.351638000	1.098501000
1	-1.553448000	6.363101000	0.430398000
1	-2.285265000	2.262479000	1.612074000
1	-2.771821000	4.694255000	1.803007000
7	-0.270382000	1.306708000	-0.244868000
7	0.815724000	2.830088000	-1.465476000
1	1.488435000	3.188311000	-2.142177000
1	0.341693000	-1.191208000	-1.820131000

**Ru-1Gd-H**



**Esol : -1584.670870**

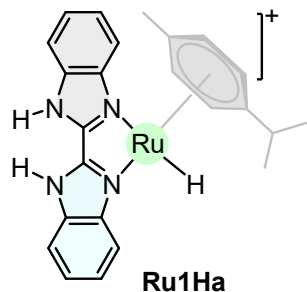
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1	-0.415796000	-3.457482000	1.446357000
6	1.044167000	-1.842041000	1.597890000
1	1.774881000	-2.359421000	0.972727000
6	1.299352000	-0.526564000	2.028958000
6	0.245630000	0.153479000	2.749593000
1	0.371839000	1.193995000	3.047157000
6	-0.931963000	-0.538864000	3.149798000
1	-1.683825000	-0.010023000	3.738798000
6	-2.374626000	-2.644745000	3.241002000
1	-3.258226000	-1.997609000	3.329367000
1	-2.146186000	-3.035715000	4.246509000
1	-2.614261000	-3.501322000	2.598120000
6	2.639523000	0.123737000	1.737268000
1	2.894994000	-0.125783000	0.692314000

6	3.704259000	-0.528296000	2.649319000
1	4.693686000	-0.102988000	2.423345000
1	3.755015000	-1.617079000	2.502468000
1	3.479159000	-0.331793000	3.709519000
6	2.658662000	1.648902000	1.894873000
1	1.871623000	2.144589000	1.309435000
1	3.627390000	2.038600000	1.550304000
1	2.539523000	1.946646000	2.948771000
44	-0.809135000	-0.515314000	0.930822000
6	-2.433070000	-0.973705000	-0.521044000
6	-3.487791000	-1.905302000	0.090426000
8	-1.285954000	-1.483611000	-0.911339000
1	-2.165913000	0.288595000	1.131760000
1	-2.996518000	-2.847020000	0.368052000
8	-4.502233000	-2.230901000	-0.871811000
1	-5.052851000	-1.430264000	-0.964864000
6	3.503817000	-2.911419000	-4.007353000
6	4.485880000	-1.898771000	-4.151585000
6	4.306922000	-0.624660000	-3.615390000
6	3.108881000	-0.369905000	-2.920486000
6	2.133160000	-1.404002000	-2.780015000
6	2.310588000	-2.685819000	-3.319731000
1	3.688311000	-3.895113000	-4.444738000
1	5.403692000	-2.127538000	-4.697804000
1	5.063053000	0.155314000	-3.726572000

1	1.555839000	-3.466050000	-3.206690000
6	1.480421000	0.455966000	-1.787363000
7	1.108998000	-0.837003000	-2.053144000
7	2.672387000	0.783847000	-2.294387000
6	0.030025000	3.483264000	-0.498378000
6	0.670098000	1.422159000	-1.070679000
6	-0.156379000	4.862634000	-0.347637000
6	-0.713248000	2.524713000	0.238852000
6	-1.119201000	5.264650000	0.577797000
1	0.424883000	5.581615000	-0.926698000
6	-1.674234000	2.948935000	1.170025000
6	-1.864813000	4.322051000	1.323083000
1	-1.300675000	6.330298000	0.730858000
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7	-0.287705000	1.243091000	-0.134845000
7	0.878714000	2.750720000	-1.301246000
1	1.569833000	3.096375000	-1.965717000
1	-3.934745000	-1.448676000	0.987235000
6	-2.995010000	0.171614000	-1.349115000
1	-2.232241000	0.944777000	-1.513970000
1	-3.265964000	-0.258512000	-2.333161000
8	-4.155432000	0.683899000	-0.679338000
1	-4.524732000	1.397462000	-1.226133000
1	0.185302000	-1.230560000	-1.805048000

### Ru1Ha



Esol -1241.364311

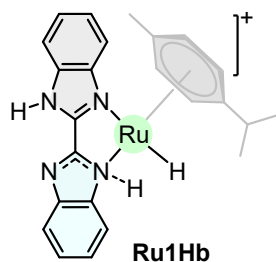
Gsol -1240.991144

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6	-0.059328000	-3.341431000	0.406087000
1	1.004162000	-3.265856000	0.635363000
6	-1.036686000	-3.076396000	1.421741000
1	-0.690992000	-2.767779000	2.412141000
6	-2.434788000	-3.204220000	1.192654000
6	-2.821103000	-3.452673000	-0.159640000
1	-3.882028000	-3.447849000	-0.420578000
6	-1.873171000	-3.735411000	-1.194492000
1	-2.216407000	-3.963238000	-2.204198000
6	0.539225000	-3.992167000	-1.985648000
1	1.480141000	-3.452243000	-1.813109000
1	0.158117000	-3.733025000	-2.982775000
1	0.758992000	-5.072651000	-1.974916000

6	-3.449172000	-2.990516000	2.299667000
1	-2.888150000	-2.618930000	3.174759000
6	-4.097666000	-4.334474000	2.686873000
1	-4.788021000	-4.196833000	3.533674000
1	-3.338199000	-5.076121000	2.978032000
1	-4.673312000	-4.748591000	1.842846000
6	-4.510562000	-1.937061000	1.939706000
1	-4.041399000	-0.973598000	1.689308000
1	-5.192548000	-1.781863000	2.789859000
1	-5.121825000	-2.251312000	1.078401000
6	-5.605658000	-1.074709000	-3.403250000
6	-6.190567000	0.213667000	-3.372230000
6	-5.662698000	1.240682000	-2.587965000
6	-4.529640000	0.930020000	-1.827230000
6	-3.940573000	-0.365986000	-1.840104000
6	-4.477735000	-1.383136000	-2.643817000
1	-6.047802000	-1.843381000	-4.040113000
1	-7.074532000	0.411655000	-3.981747000
1	-6.107354000	2.236847000	-2.568402000
1	-4.018238000	-2.370723000	-2.678971000
6	-2.765884000	0.890846000	-0.481212000
7	-2.849708000	-0.360010000	-0.984657000
7	-3.760401000	1.692932000	-0.963378000
6	-0.106877000	1.838573000	1.800528000
6	-1.679872000	1.112725000	0.413951000
6	0.737651000	2.556030000	2.655581000
6	0.119227000	0.468201000	1.487707000

6	1.824539000	1.861643000	3.189459000
1	0.555791000	3.606155000	2.888769000
6	1.221352000	-0.211898000	2.027735000
6	2.064388000	0.502098000	2.878333000
1	2.510000000	2.383030000	3.860554000
1	1.411546000	-1.255590000	1.778713000
1	2.932198000	0.002793000	3.313709000
7	-0.882674000	0.043128000	0.628455000
7	-1.246396000	2.208489000	1.103965000
1	-3.905462000	2.675693000	-0.744737000
1	-1.686088000	3.125674000	1.120574000
1	-0.558026000	-1.111431000	-1.550086000

### Ru1Hb



**Esol -1241.326614**

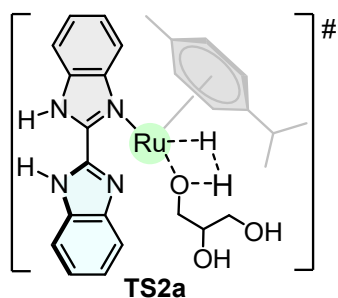
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6	-0.349372000	-3.717315000	-0.260230000

1	0.691895000	-3.920462000	-0.514707000
6	-0.672045000	-3.151327000	0.998578000
1	0.140246000	-2.907854000	1.687854000
6	-2.038412000	-2.911670000	1.424348000
6	-3.053256000	-3.128565000	0.481792000
1	-4.091530000	-2.891064000	0.714830000
6	-2.714504000	-3.544161000	-0.857859000
1	-3.511683000	-3.620449000	-1.600644000
6	-1.089631000	-4.514916000	-2.584771000
1	-0.084185000	-4.239496000	-2.931244000
1	-1.822164000	-4.194142000	-3.338381000
1	-1.137361000	-5.614815000	-2.517510000
6	-2.281517000	-2.409749000	2.834058000
1	-1.453599000	-1.715271000	3.066455000
6	-2.177161000	-3.597313000	3.815133000
1	-2.271376000	-3.239503000	4.851849000
1	-1.212713000	-4.119246000	3.719678000
1	-2.982011000	-4.325610000	3.625877000
6	-3.602133000	-1.652458000	3.012005000
1	-3.697959000	-0.826368000	2.290774000
1	-3.650871000	-1.226104000	4.025081000
1	-4.471668000	-2.318662000	2.893038000
6	-4.798292000	-0.903548000	-4.541112000
6	-5.477110000	0.338061000	-4.472063000
6	-5.205252000	1.271356000	-3.471531000
6	-4.228876000	0.915790000	-2.532880000
6	-3.543048000	-0.331722000	-2.591420000

6	-3.826893000	-1.257272000	-3.607540000
1	-5.042910000	-1.596983000	-5.348075000
1	-6.232245000	0.572259000	-5.224985000
1	-5.724699000	2.229290000	-3.421872000
1	-3.293365000	-2.206591000	-3.662373000
6	-2.763190000	0.778896000	-0.879274000
7	-2.645870000	-0.385933000	-1.538049000
7	-3.709775000	1.582529000	-1.434464000
6	-1.109712000	1.267385000	2.248387000
6	-1.927378000	0.981411000	0.277564000
6	-0.890731000	1.655593000	3.576097000
6	-0.199976000	0.402423000	1.595766000
6	0.261474000	1.172003000	4.205108000
1	-1.595318000	2.311126000	4.090502000
6	0.956727000	-0.070993000	2.205340000
6	1.171095000	0.331252000	3.531950000
1	0.463822000	1.451614000	5.240944000
1	1.655722000	-0.728077000	1.685838000
1	2.060573000	-0.022894000	4.056559000
7	-0.733195000	0.169390000	0.295174000
7	-2.176942000	1.598932000	1.397627000
1	-3.956831000	2.515769000	-1.110988000
1	-0.394758000	-1.438470000	-1.779538000
1	-0.087598000	0.317825000	-0.492315000

**TS2a**



**Esol -1585.829918**

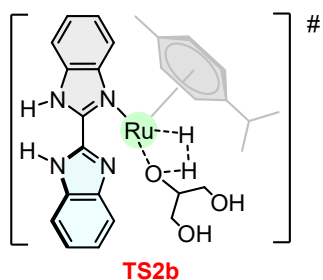
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1	-15.717533000	-2.088560000	-2.516489000
6	-15.771958000	-1.875981000	-0.339938000
1	-15.313725000	-2.848664000	-0.158949000
6	-16.058085000	-1.031077000	0.762097000
6	-16.529905000	0.301121000	0.483074000
1	-16.682169000	1.007490000	1.298873000
6	-16.732302000	0.738063000	-0.849531000
1	-17.042899000	1.768544000	-1.033208000
6	-16.789735000	0.322686000	-3.369743000
1	-16.290869000	-0.307225000	-4.118440000
1	-16.483083000	1.367709000	-3.517814000
1	-17.875803000	0.264352000	-3.551699000
6	-15.850754000	-1.549294000	2.171683000
1	-14.906874000	-2.120263000	2.143667000
6	-17.001466000	-2.524022000	2.505785000
1	-16.847018000	-2.953046000	3.507799000

1	-17.055717000	-3.351584000	1.782542000
1	-17.971722000	-2.001058000	2.504015000
6	-15.735302000	-0.458497000	3.243259000
1	-14.949395000	0.273333000	3.006911000
1	-15.484726000	-0.921104000	4.209534000
1	-16.684411000	0.085464000	3.378335000
44	-14.651117000	0.044072000	-0.678828000
6	-12.611981000	-1.424113000	-2.547724000
1	-14.059799000	1.448388000	-1.542077000
1	-13.172650000	-2.352223000	-2.323578000
6	-13.056721000	-0.878500000	-3.899955000
1	-14.113801000	-0.553740000	-3.823452000
6	-12.181696000	1.909773000	2.365219000
6	-12.324905000	-0.083583000	1.366451000
6	-11.859749000	3.033279000	3.135529000
6	-13.288000000	1.887713000	1.477842000
6	-12.683120000	4.149553000	2.983029000
1	-11.008555000	3.033239000	3.818024000
6	-14.101557000	3.021664000	1.328496000
6	-13.782359000	4.144249000	2.092169000
1	-12.471964000	5.050006000	3.563250000
1	-14.947760000	3.020629000	0.640229000
1	-14.396200000	5.042620000	2.001384000
7	-13.346096000	0.633769000	0.872974000
7	-11.599537000	0.659380000	2.257096000
1	-10.830626000	0.306005000	2.823169000
8	-12.715579000	-0.490246000	-1.488220000

1	-13.406798000	0.793109000	-1.730424000
1	-11.538575000	-1.691823000	-2.614495000
8	-12.241424000	0.262115000	-4.216342000
1	-12.437219000	0.467370000	-5.150362000
8	-13.373631000	-1.277106000	-6.220261000
1	-13.042360000	-1.798194000	-6.969720000
6	-12.961854000	-1.927451000	-5.000908000
1	-13.621789000	-2.783043000	-4.768445000
1	-11.920722000	-2.287913000	-5.084924000
6	-10.683212000	-3.173168000	0.460907000
6	-11.974740000	-1.456666000	1.022343000
6	-9.675893000	-4.071935000	0.087366000
6	-12.050287000	-3.558062000	0.579133000
6	-10.076849000	-5.386430000	-0.163211000
1	-8.632910000	-3.763432000	-0.004200000
6	-12.428579000	-4.889927000	0.330040000
6	-11.429435000	-5.789164000	-0.043108000
1	-9.326992000	-6.123475000	-0.458982000
1	-13.472382000	-5.198271000	0.420515000
1	-11.691819000	-6.829270000	-0.249148000
7	-12.827427000	-2.468263000	0.939510000
7	-10.666869000	-1.827132000	0.776772000
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**TS2b**



**Esol : -1585.828111**

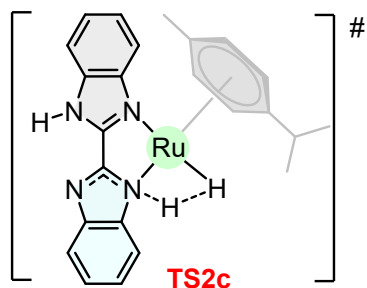
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6	-15.777037000	-1.890745000	-0.386653000
1	-15.326841000	-2.872041000	-0.233858000
6	-16.026446000	-1.062444000	0.736462000
6	-16.483332000	0.281632000	0.491601000
1	-16.603943000	0.976214000	1.322761000
6	-16.711941000	0.744938000	-0.827326000
1	-17.014166000	1.782100000	-0.985952000
6	-16.847137000	0.374180000	-3.349322000
1	-16.404986000	-0.264953000	-4.124904000
1	-16.505851000	1.408512000	-3.497370000
1	-17.941106000	0.361448000	-3.487419000
6	-15.800597000	-1.608890000	2.132442000
1	-14.870843000	-2.200017000	2.075098000
6	-16.965946000	-2.562982000	2.475210000
1	-16.799603000	-3.012640000	3.466216000

1	-17.054509000	-3.376393000	1.739439000
1	-17.923804000	-2.018399000	2.503525000
6	-15.637862000	-0.539573000	3.219620000
1	-14.842593000	0.180397000	2.978228000
1	-15.375203000	-1.024100000	4.171806000
1	-16.571897000	0.021561000	3.385758000
44	-14.638075000	0.017443000	-0.720127000
6	-12.664307000	-1.393658000	-2.707288000
1	-14.046923000	1.425427000	-1.584492000
1	-13.273277000	-2.311581000	-2.571127000
6	-13.149562000	-0.712788000	-3.986092000
1	-14.233195000	-0.519506000	-3.906380000
6	-12.179987000	1.899196000	2.318054000
6	-12.313184000	-0.112618000	1.352511000
6	-11.869223000	3.033799000	3.076540000
6	-13.259086000	1.870147000	1.398458000
6	-12.675905000	4.154982000	2.878448000
1	-11.038223000	3.038345000	3.783409000
6	-14.056156000	3.009139000	1.204041000
6	-13.748125000	4.143091000	1.955326000
1	-12.472580000	5.064460000	3.447258000
1	-14.880752000	3.004263000	0.490228000
1	-14.349526000	5.045506000	1.828689000
7	-13.312864000	0.605184000	0.815671000
7	-11.607902000	0.641968000	2.251700000
1	-10.869874000	0.290965000	2.858857000
8	-12.737460000	-0.555338000	-1.566098000

1	-13.401288000	0.777988000	-1.777749000
8	-12.436149000	0.525708000	-4.150691000
1	-12.797681000	0.967851000	-4.936179000
6	-10.632742000	-3.239336000	0.689818000
6	-11.956014000	-1.492284000	1.055823000
6	-9.601764000	-4.158353000	0.455783000
6	-12.011169000	-3.597621000	0.626086000
6	-9.991443000	-5.466679000	0.160579000
1	-8.550503000	-3.868141000	0.498943000
6	-12.378415000	-4.924229000	0.334393000
6	-11.355740000	-5.843765000	0.102516000
1	-9.223555000	-6.219476000	-0.030652000
1	-13.430671000	-5.212307000	0.285340000
1	-11.607982000	-6.880210000	-0.132419000
7	-12.807615000	-2.490960000	0.869245000
7	-10.632559000	-1.889651000	0.988746000
1	-9.817717000	-1.279529000	0.986160000
1	-12.978261000	-1.393523000	-4.839133000
6	-11.194338000	-1.829736000	-2.801728000
1	-10.900403000	-2.264141000	-1.831627000
1	-10.563133000	-0.946377000	-3.003981000
8	-11.081962000	-2.803125000	-3.856054000
1	-10.152112000	-3.080675000	-3.897387000

**TS2c**



**Esol : -1241.313020**

**Gsol : -1240.945611**

44	-1.374335000	-1.811727000	-0.426544000
6	-0.660647000	-3.835150000	-1.097060000
6	-0.109063000	-3.548128000	0.193997000
1	0.972520000	-3.545221000	0.333018000
6	-0.963464000	-3.166654000	1.265174000
1	-0.513125000	-2.856488000	2.211505000
6	-2.397087000	-3.138853000	1.143107000
6	-2.922993000	-3.418415000	-0.141699000
1	-3.993374000	-3.305863000	-0.322381000
6	-2.077068000	-3.753966000	-1.252128000
1	-2.514478000	-3.937126000	-2.233501000
6	0.223492000	-4.206103000	-2.250177000
1	1.212638000	-3.737380000	-2.163762000
1	-0.228956000	-3.920490000	-3.209052000
1	0.363692000	-5.299891000	-2.250995000
6	-3.254446000	-2.763149000	2.334177000
1	-2.629708000	-2.116463000	2.975246000
6	-3.596292000	-4.037717000	3.133530000

1	-4.161014000	-3.773768000	4.040668000
1	-2.688031000	-4.579135000	3.439093000
1	-4.215574000	-4.719113000	2.528146000
6	-4.518025000	-1.977713000	1.958425000
1	-4.275149000	-1.091827000	1.352111000
1	-5.027844000	-1.638650000	2.872258000
1	-5.234619000	-2.597139000	1.395884000
6	-5.457180000	-0.978470000	-3.640259000
6	-6.066164000	0.293788000	-3.534120000
6	-5.573319000	1.271405000	-2.668258000
6	-4.451012000	0.927048000	-1.907501000
6	-3.833728000	-0.352814000	-2.000205000
6	-4.338700000	-1.320718000	-2.880637000
1	-5.872672000	-1.709844000	-4.336163000
1	-6.940959000	0.518527000	-4.147361000
1	-6.036079000	2.255903000	-2.586015000
1	-3.866311000	-2.297717000	-2.975503000
6	-2.715821000	0.832867000	-0.529109000
7	-2.760237000	-0.379214000	-1.119877000
7	-3.713539000	1.638763000	-0.973650000
6	-0.325143000	1.743585000	1.943838000
6	-1.676223000	1.087267000	0.424404000
6	0.369190000	2.447899000	2.942916000
6	0.125863000	0.450200000	1.538005000
6	1.493418000	1.840704000	3.504020000
1	0.033527000	3.437316000	3.260536000
6	1.256005000	-0.156890000	2.094641000

6	1.931285000	0.561772000	3.085105000
1	2.052440000	2.362576000	4.283739000
1	1.598199000	-1.140931000	1.770052000
1	2.817765000	0.124305000	3.549301000
7	-0.763411000	0.036072000	0.548041000
7	-1.459321000	2.115613000	1.226950000
1	-3.872564000	2.596128000	-0.666172000
1	-0.305660000	-1.103926000	-1.515556000
1	-0.285617000	-0.418473000	-0.597523000

## 7. References

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<sup>1</sup> Gaussian 09, Revision *D.01*, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.